Ab initio nuclear structure with chiral interactions

James P. Vary
Iowa State University

International School of Nuclear Physics
Erice-Sicily, Italy
September 16-24, 2011

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

QCD
Theory of strong interactions

χEFT
Chiral Effective Field Theory

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

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

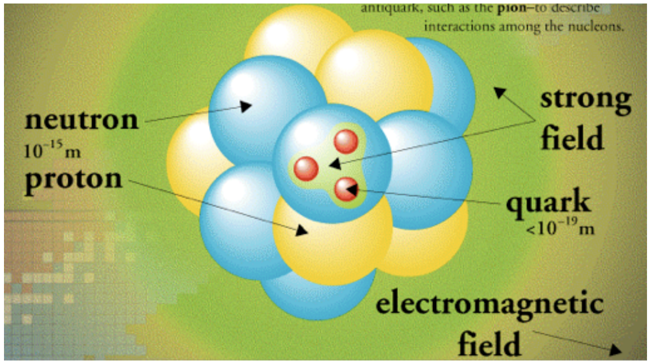
Big Bang
Nucleosynthesis
& Stellar Reactions

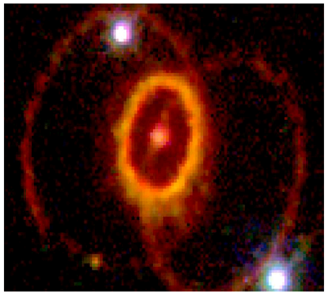
Density Functional Theory
improved functionals
remove computationally-imposed constraints
properties for all nuclei with A>16

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





www.unedf.org

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 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 fm^{-1})

"Consistent" NNN and higher-body forces, as well as electroweak
currents, 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!

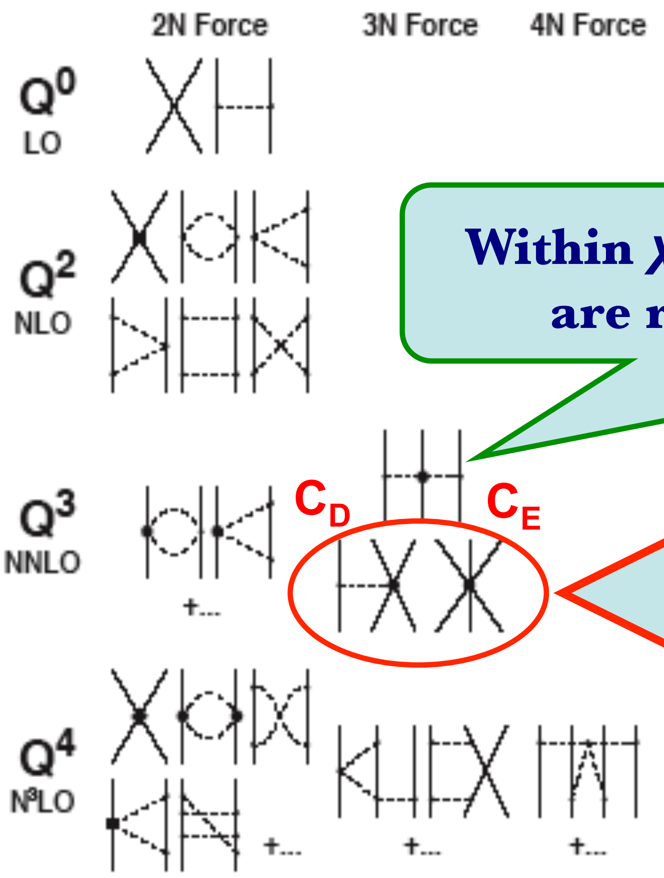
Effective Nucleon Interaction

(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

Regularization is essential, which is obvious within the Harmonic Oscillator wave function basis.

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 bookkeepping of anti-symmetrization)
- Diagonalize this sparse many-body H in its “m-scheme” basis where [α =(n,l,j,$m_{j,}\tau_z$)]

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

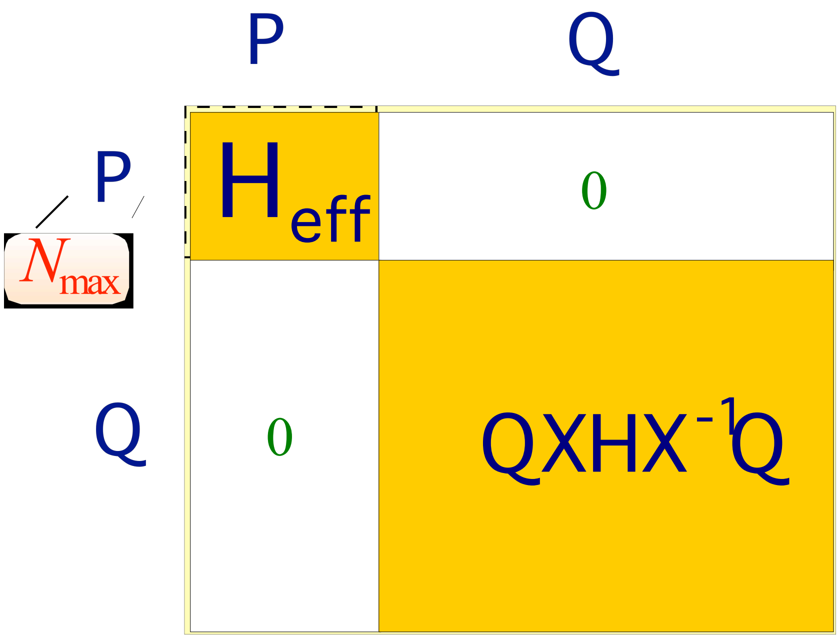
$$n = 1,2,\ldots,10^{10} \text{ or more!}$$

- 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

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



$$\begin{array}{c|cc} & P & Q \\ \hline P & H_{\text{eff}} & 0 \\ Q & 0 & QXHX^{-1}Q \end{array}$$

$N_{\max}$

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

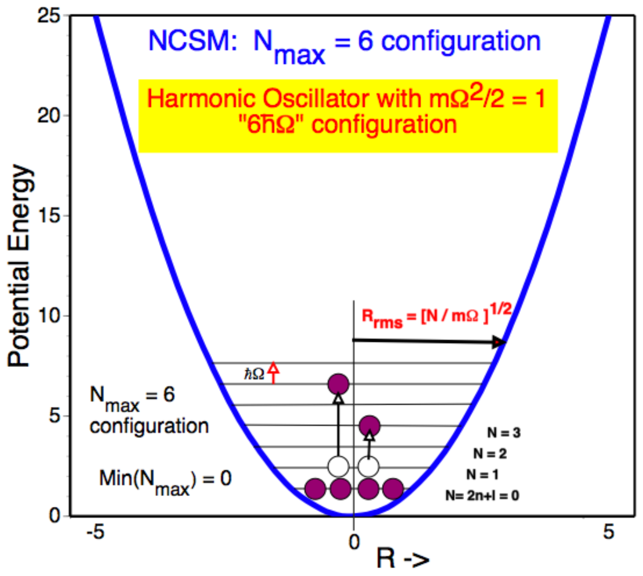
$$H_{\text{eff}}: \quad E_1, E_2, E_3, \ldots E_{d_P}$$

model space dimension

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

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

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



PRL 99, 042501 (2007) PHYSICAL REVIEW LETTERS week ending 27 JULY 2007

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”

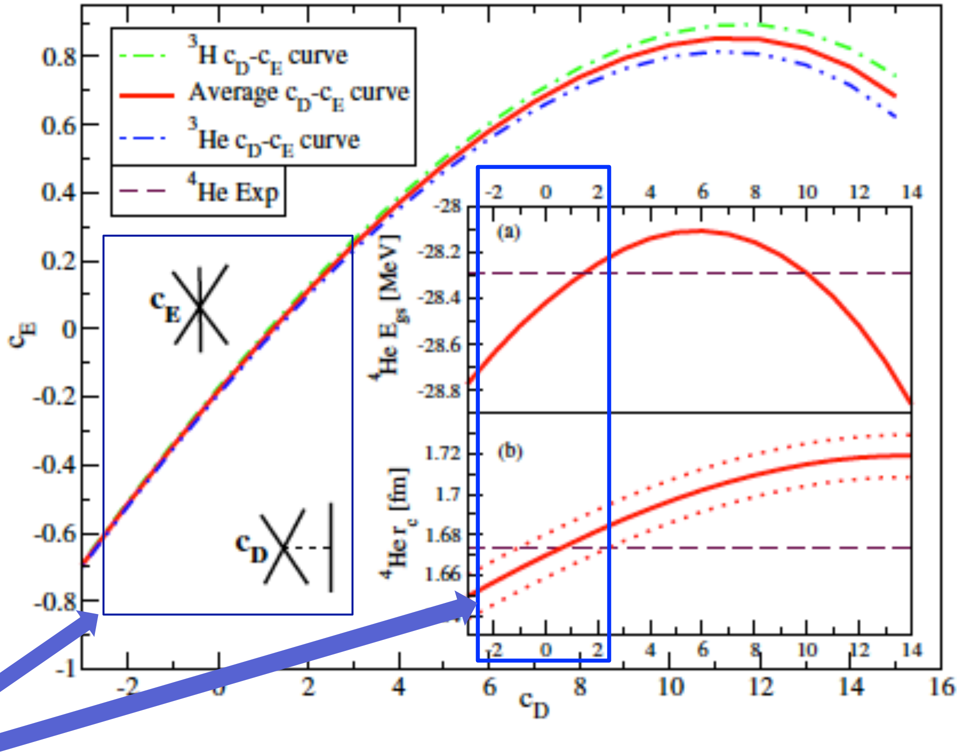
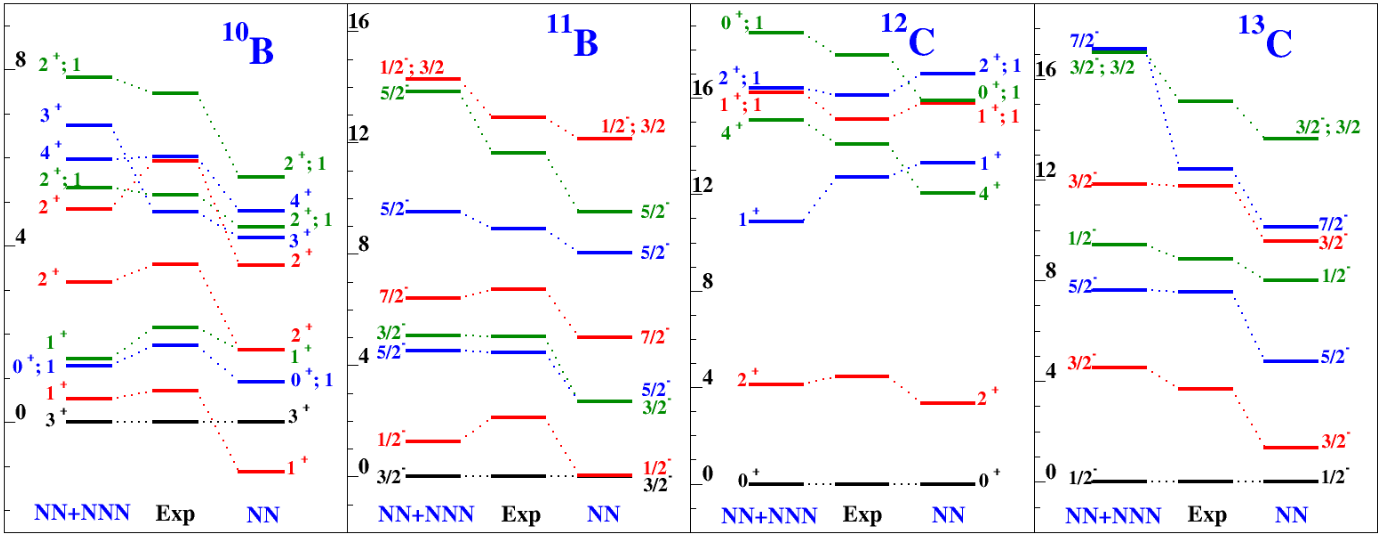


FIG. 1 (color online). Relations between c_D and c_E for which the binding energy of ^{3}H (8.482 MeV) and ^{3}He (7.718 MeV) are reproduced. (a) ^{4}He ground-state energy along the averaged curve. (b) ^{4}He charge radius r_c along the averaged curve. Dotted lines represent the r_c uncertainty due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

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*



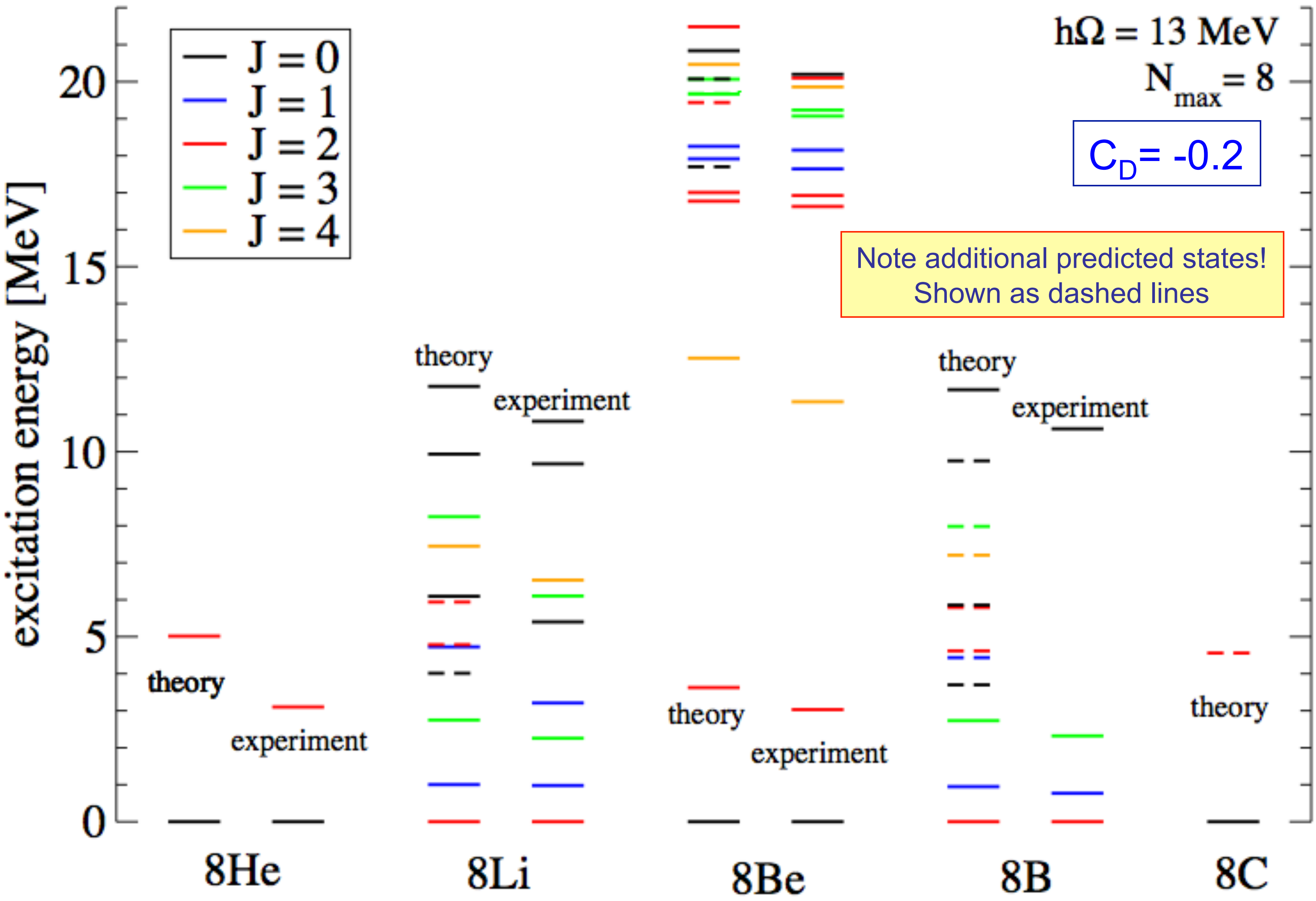
P. Navratil, V.G. Gueorguiev,
J. P. Vary, W. E. Ormand
and A. Nogga,
PRL 99, 042501(2007);
ArXiV: nucl-th 0701038.

$c_D = -1$

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)*

spectrum A=8 nuclei with N3LO 2-body + N2LO 3-body



C_D= -0.2

Note additional predicted states!
Shown as dashed lines

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

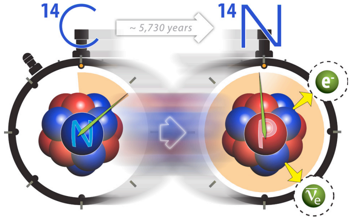
PRL 106, 202502 (2011) PHYSICAL REVIEW LETTERS week ending 20 MAY 2011

Origin of the Anomalous Long Lifetime of ^{14}C

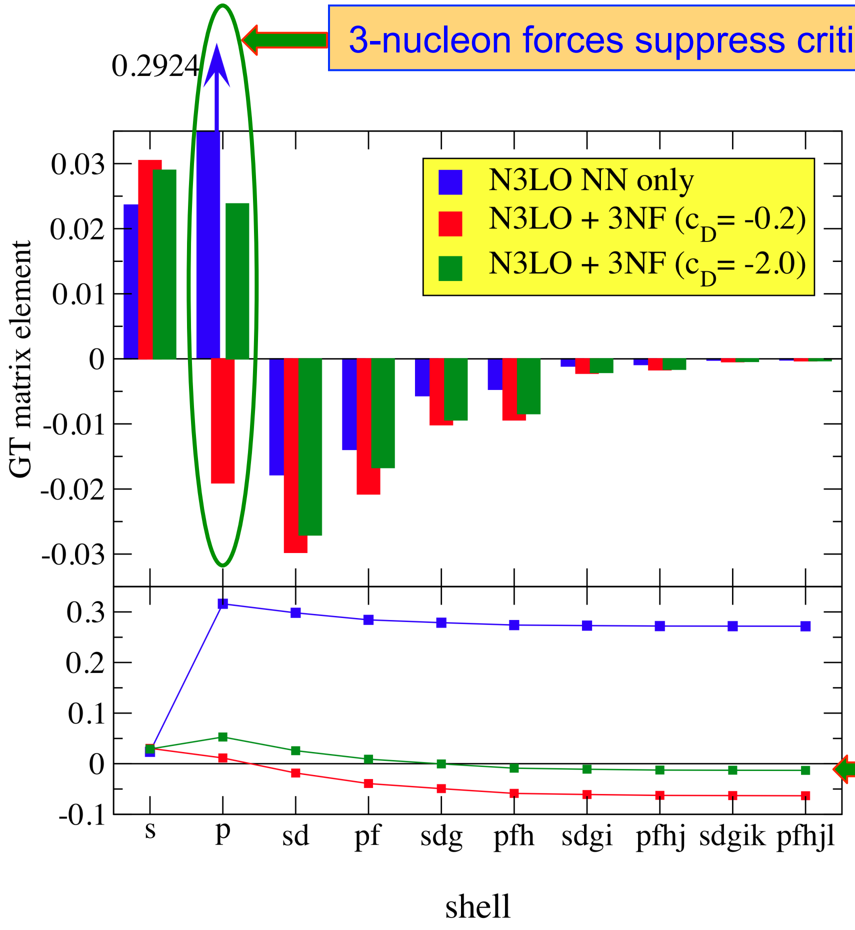
P. Maris,[1] J.P. Vary,[1] P. Navrátil,[2,3] W.E. Ormand,[3,4] H. Nam,[5] and D.J. Dean[5]

- Solves the puzzle of the long but useful lifetime of ^{14}C
- Establishes a major role for strong 3-nucleon forces in nuclei
- Strengthens foundation for guiding DOE-supported experiments

---



3-nucleon forces suppress critical component



net decay rate
Is very small

- Dimension of matrix solved for 8 lowest states ~ 1x10^9
- Solution takes ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL
- "Scaling of *ab initio* nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97 (2010)

Detailed results and estimated corrections due to chiral 2-body currents

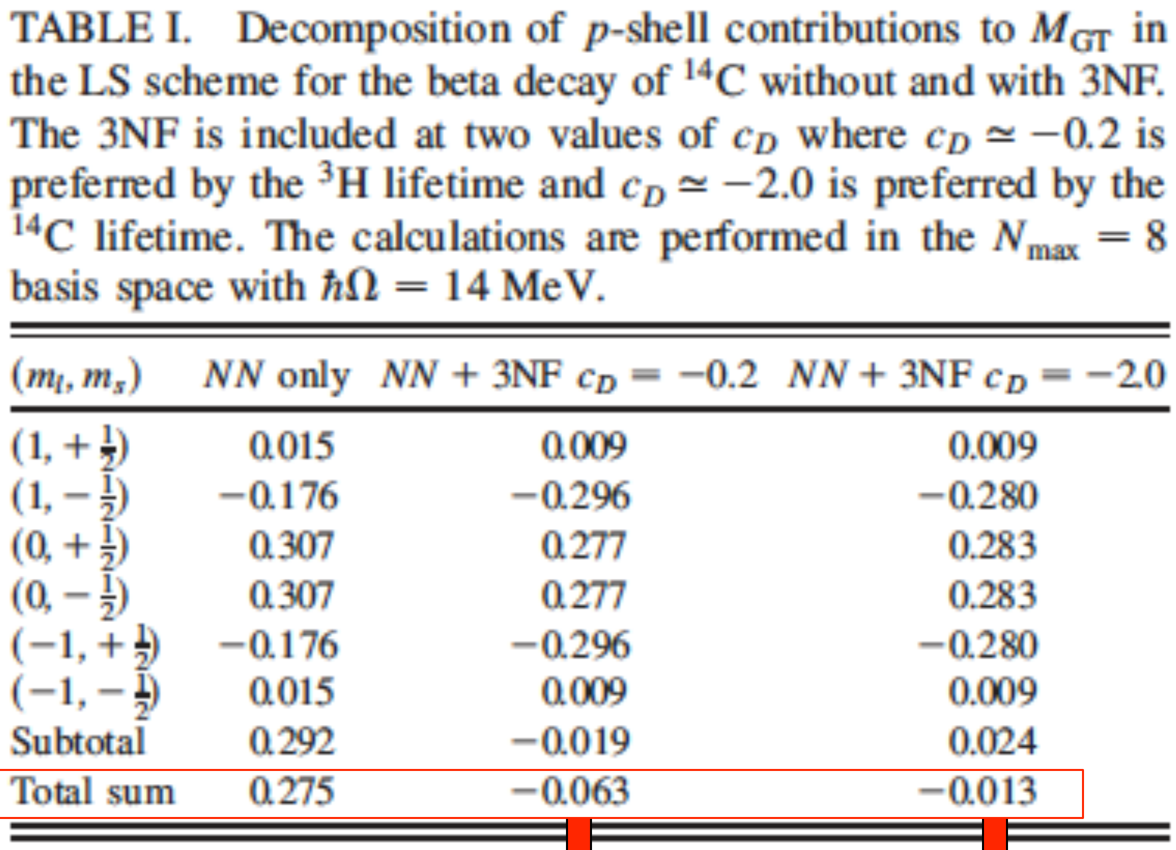


TABLE I. Decomposition of p-shell contributions to M_{GT} in the LS scheme for the beta decay of ^{14}C without and with 3NF. The 3NF is included at two values of c_D where $c_D \simeq -0.2$ is preferred by the ^{3}H lifetime and $c_D \simeq -2.0$ is preferred by the ^{14}C lifetime. The calculations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

Tritium half-life

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

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

Preliminary

*J. Menéndez, D. Gazit and A. Schwenk, PRL (to appear); arXiv 1103.3622; (estimated using their effective 1-body quenching approximation)

Innovations underway to improve the NCSM with aims:
(1) improve treatment of clusters and intruders
(2) enable *ab initio* solutions of heavier nuclei
Initially, all follow the NCFC approach = extrapolations

Importance Truncated – NCSM
Extrapolate full basis at each Nmax using a sequence with improving tolerance
Robert Roth and collaborators

“Realistic” single-particle basis - Woods-Saxon example
Control the spurious CM motion with Lagrange multiplier term
A. Negoita, ISU PhD thesis project
Alternative sp basis spaces – Mark Caprio collaboration

SU(3) No Core Shell Model
Add symmetry-adapted many-body basis states
Preserve exactly the CM factorization
LSU - ISU – OSU collaboration

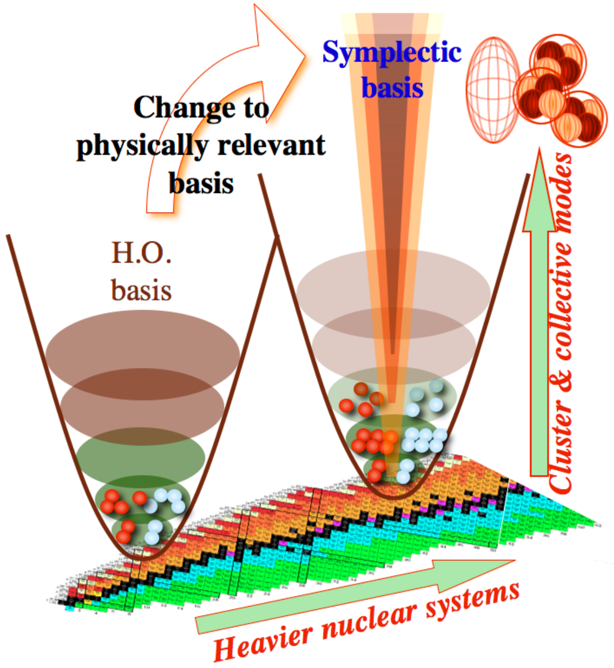
No Core Monte Carlo Shell Model
Invokes single particle basis (FCI) truncation
Separate spurious CM motion in same way as CC approach
Scales well to larger nuclei
U. Tokyo - ISU collaboration

Taming the scale explosion in nuclear calculations
NSF PetaApps - Louisiana State, Iowa State, Ohio State collaboration

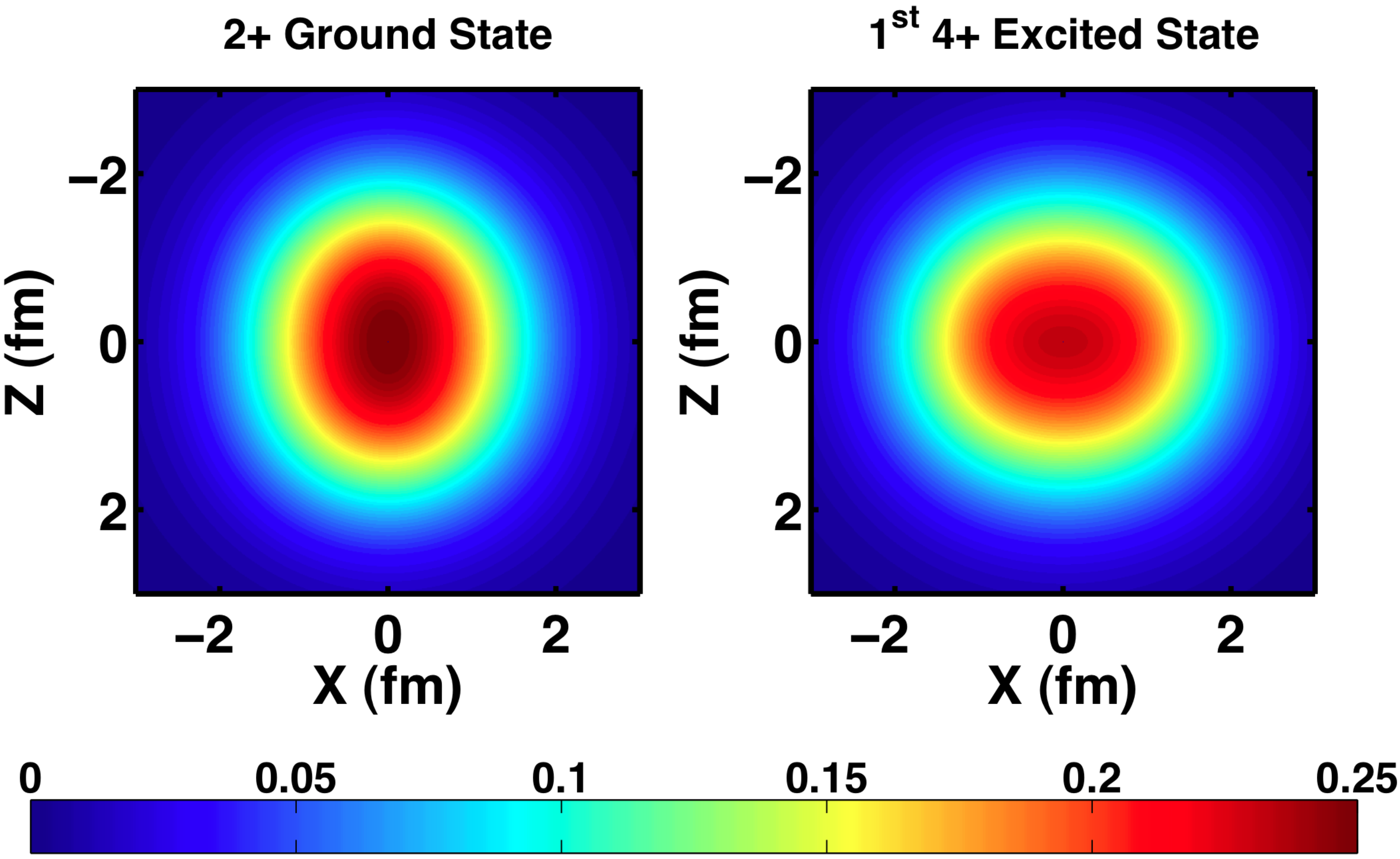
- Goals
  - Ab initio calculations of nuclei with unprecedented accuracy using basis-space expansions
  - Current calculations limited to nuclei with A ≤ 16 (up to 20 billion basis states with 2-body forces)

- 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



^{8}Li translationally invariant 1-body density distributions



Chase Cockrell, ISU PhD student

Alternative renormalization scheme - SRG

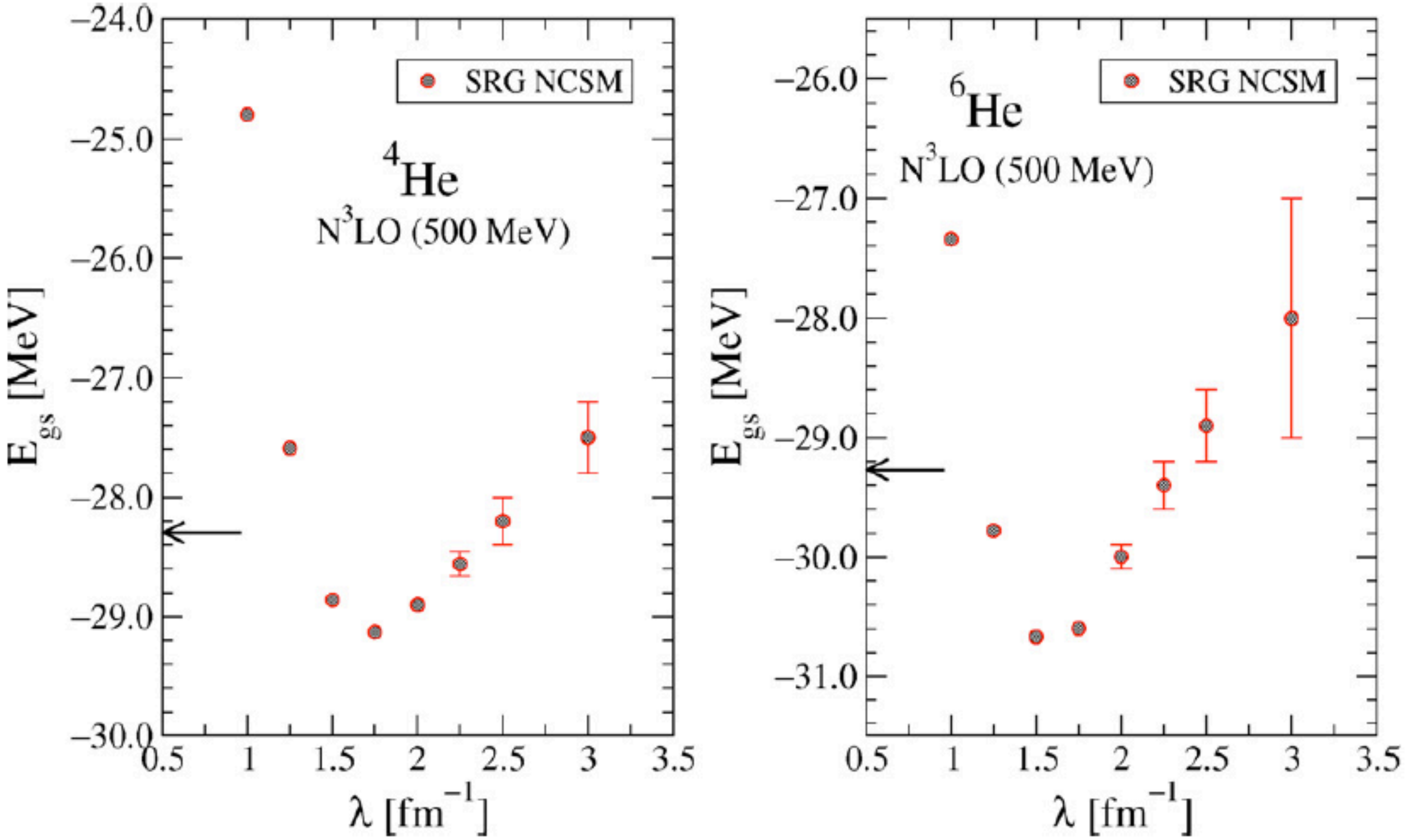
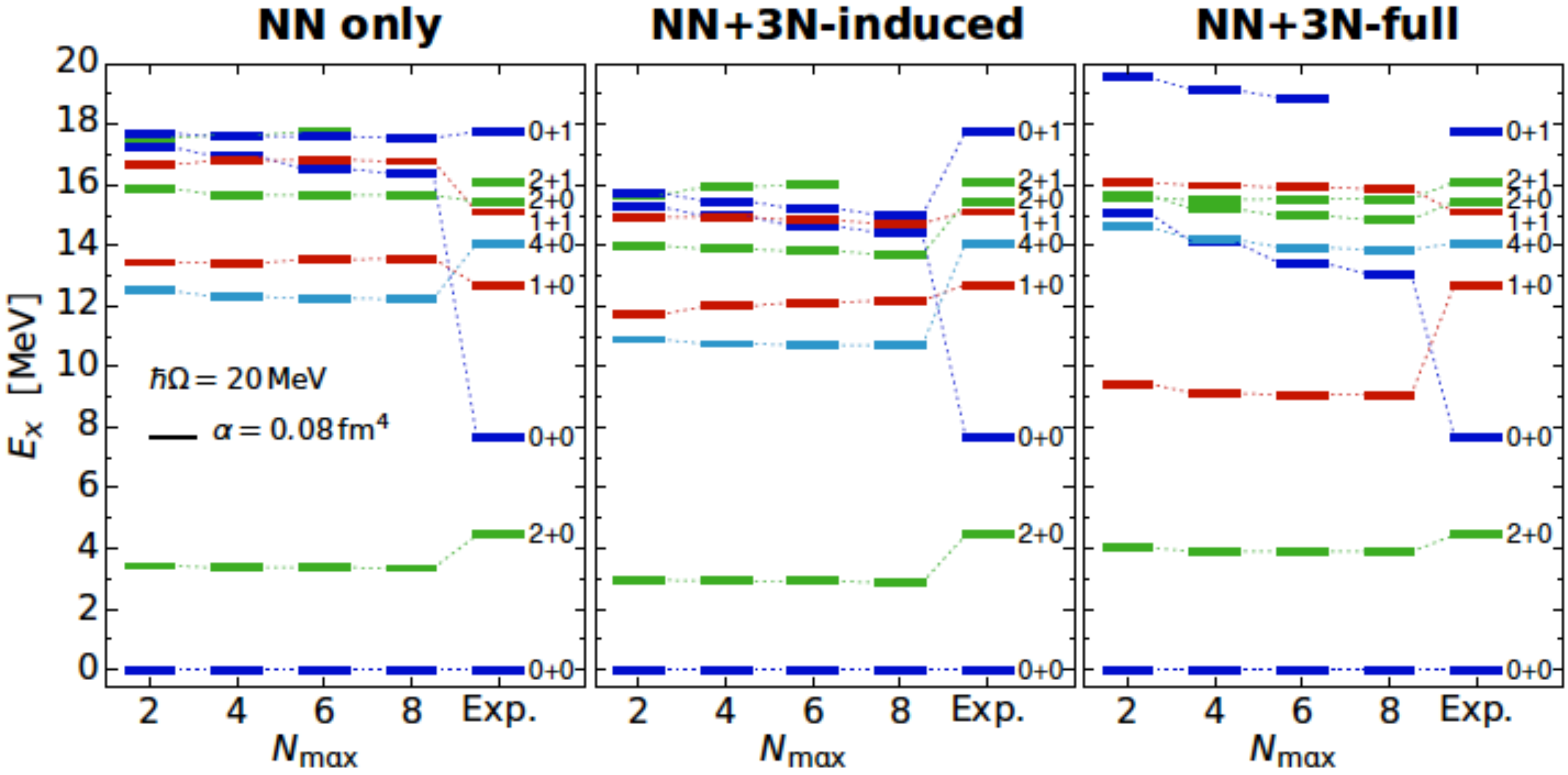


Fig. 15. Plot of the ground-state energy of ^{4}He and ^{6}He vs. λ for potentials evolved by the SRG from the 500 MeV N^{3}LO *NN*-only potential from Ref. [13]. Conservative error bars have been included with the larger λ's, for which an extrapolation is needed. The arrow marks the experimental binding.

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

R.Roth: Include 3NF within SRG renormalization



- IT-NCSM gives access to **complete spectroscopy of p- and sd-shell nuclei** starting from chiral NN+3N interactions

Descriptive Science

↓

Predictive Science

“Proton-Dripping Fluorine-14”

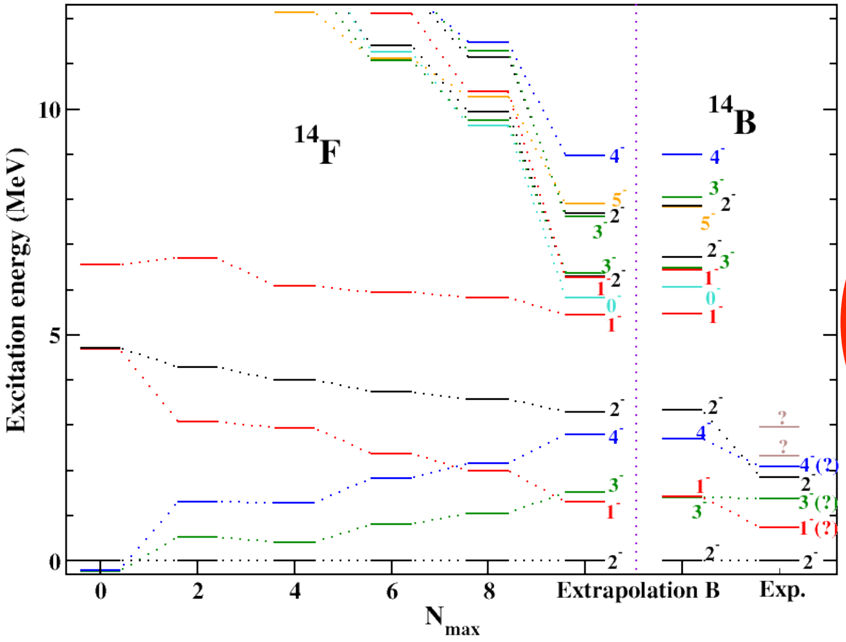
Objectives

- Apply *ab initio* microscopic nuclear theory’s predictive power to major test case

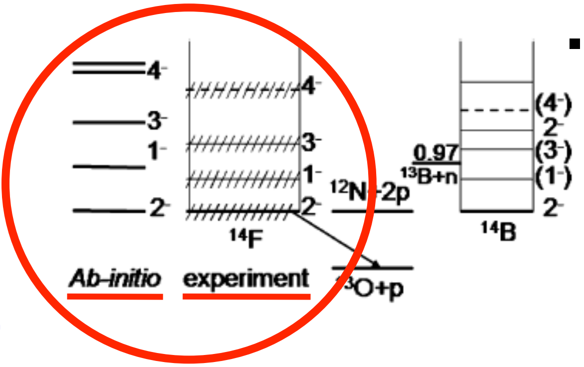
Impact

- Deliver robust predictions important for improved energy sources
- Provide important guidance for DOE-supported experiments
- Compare with new experiment to improve theory of strong interactions

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



Experiment confirms our published predictions!



V.Z. Goldberg et al.,
Phys. Lett. B 692, 307 (2010)

- Dimension of matrix solved for 14 lowest states ~ $2\text{x}10^9$
- Solution takes ~ 2.5 hours on 30,000 cores (Cray XT4 Jaguar at ORNL)
- “Scaling of ab-initio nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97 (2010)

Ab Initio Neutron drops in traps

↓

UNEDF

Properties of trapped neutrons interacting with realistic nuclear Hamiltonians

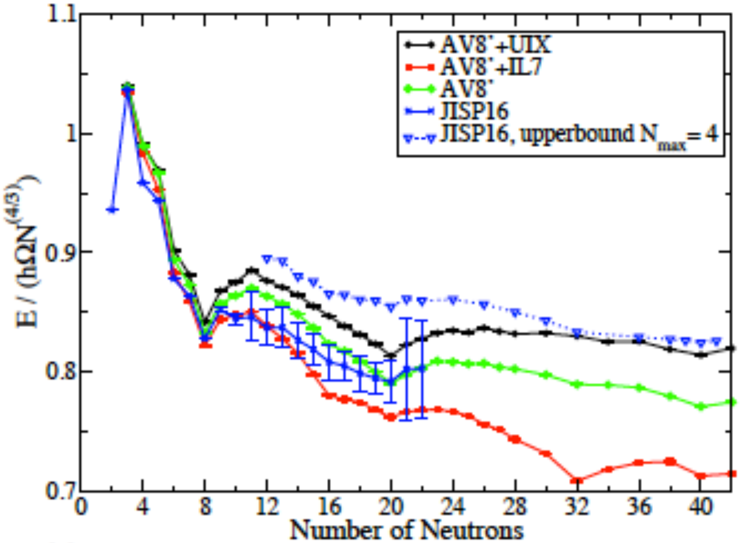
J. Carlson and S. Gandolfi
Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545

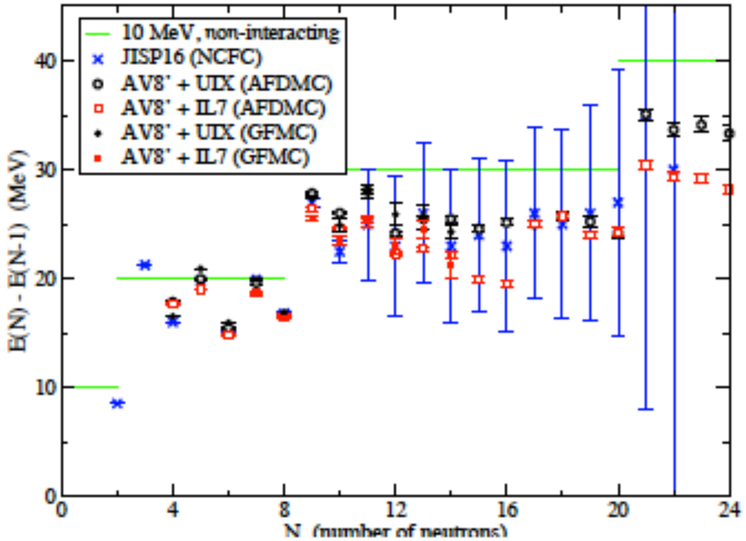
Pieter Maris and James Vary
Iowa State University, Ames, Iowa, 50011

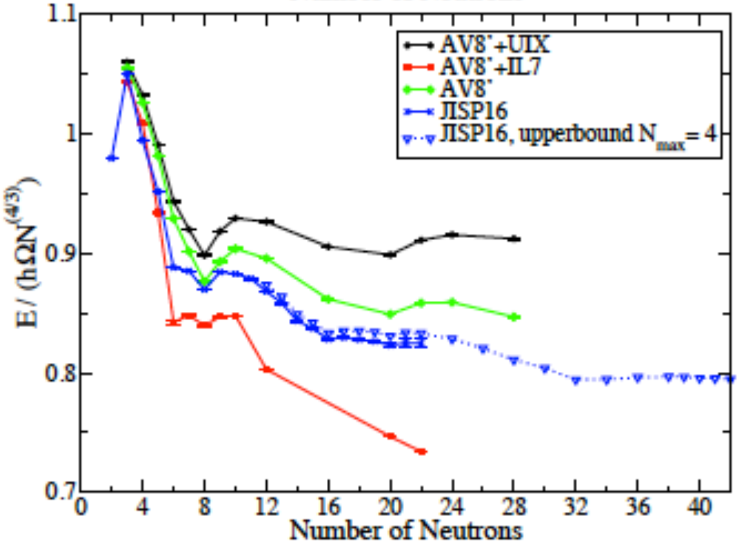
Steven C. Pieper
Physics Division, Argonne National Laboratory, Argonne, IL 61801

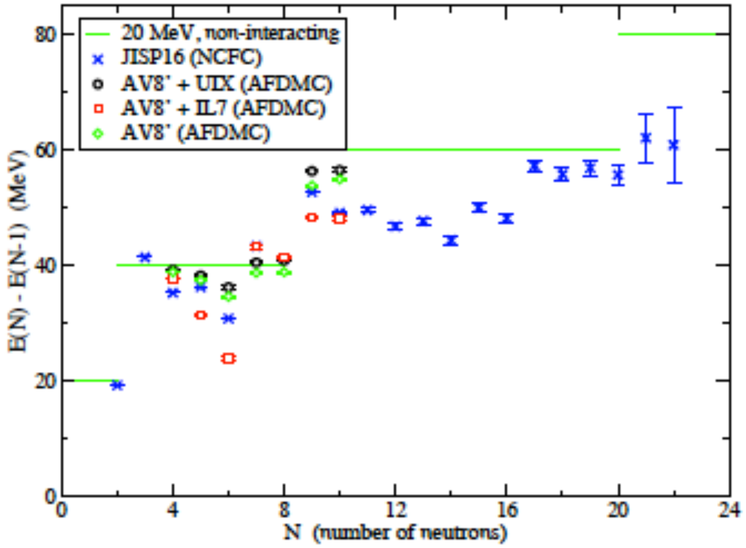
(Dated: April 20, 2011)

Preliminary









Ab initio Nuclear Structure

↓

Ab initio Nuclear Reactions

NCSM/RGM

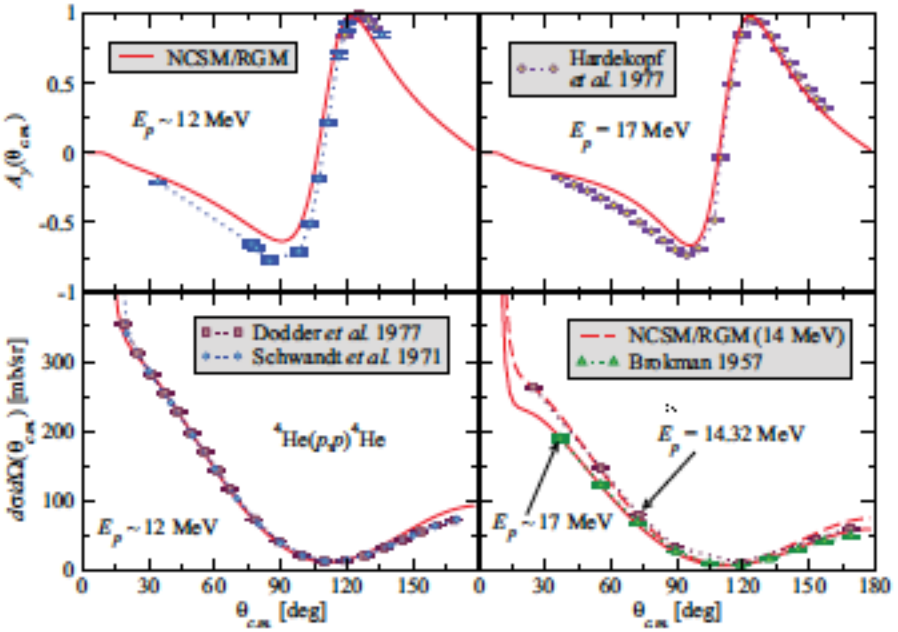


Figure 7. *Calculated p-^{4}He differential cross section (bottom panels) and analyzing power (top panels) for proton laboratory energies Ep = 12, 14.32 and 17 MeV compared to experimental data from Refs. [29, 30, 31, 32]. The SRG-N^{3}LO NN potential with $\lambda = 2.02$ fm^{-1} was used.*

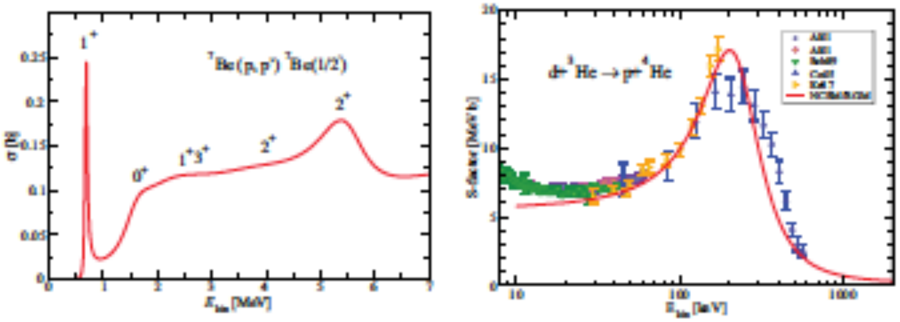


Figure 8. *Calculated inelastic ^{7}Be(p,p′)^{7}Be(1/2$^-$) cross section with indicated positions of the P-wave resonances (left figure). Calculated S-factor of the ^{3}He(d,p)^{4}He fusion reaction compared to experimental data (right figure). Energies are in the center of mass. The SRG-N^{3}LO NN potential with $\lambda = 1.85$ fm^{-1} ($\lambda = 1.5$ fm^{-1}) was used, respectively.*

P. Navrátil, R. Roth, and S. Quaglioni, *Phys. Rev. C 82 (2010)* 034609

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

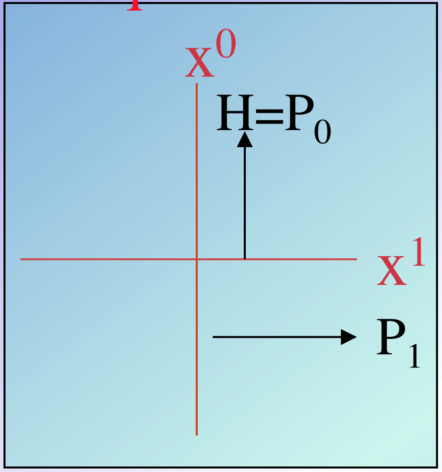
J. P. Vary, H. Honkanen, Jun Li, P. Maris, S. J. Brodsky, A. Harindranath,
G. F. de Teramond, P. Sternberg, E. G. Ng and C. Yang,
"Hamiltonian light-front field theory in a basis function approach",
Phys. Rev. C 81, 035205 (2010); arXiv nucl-th 0905.1411

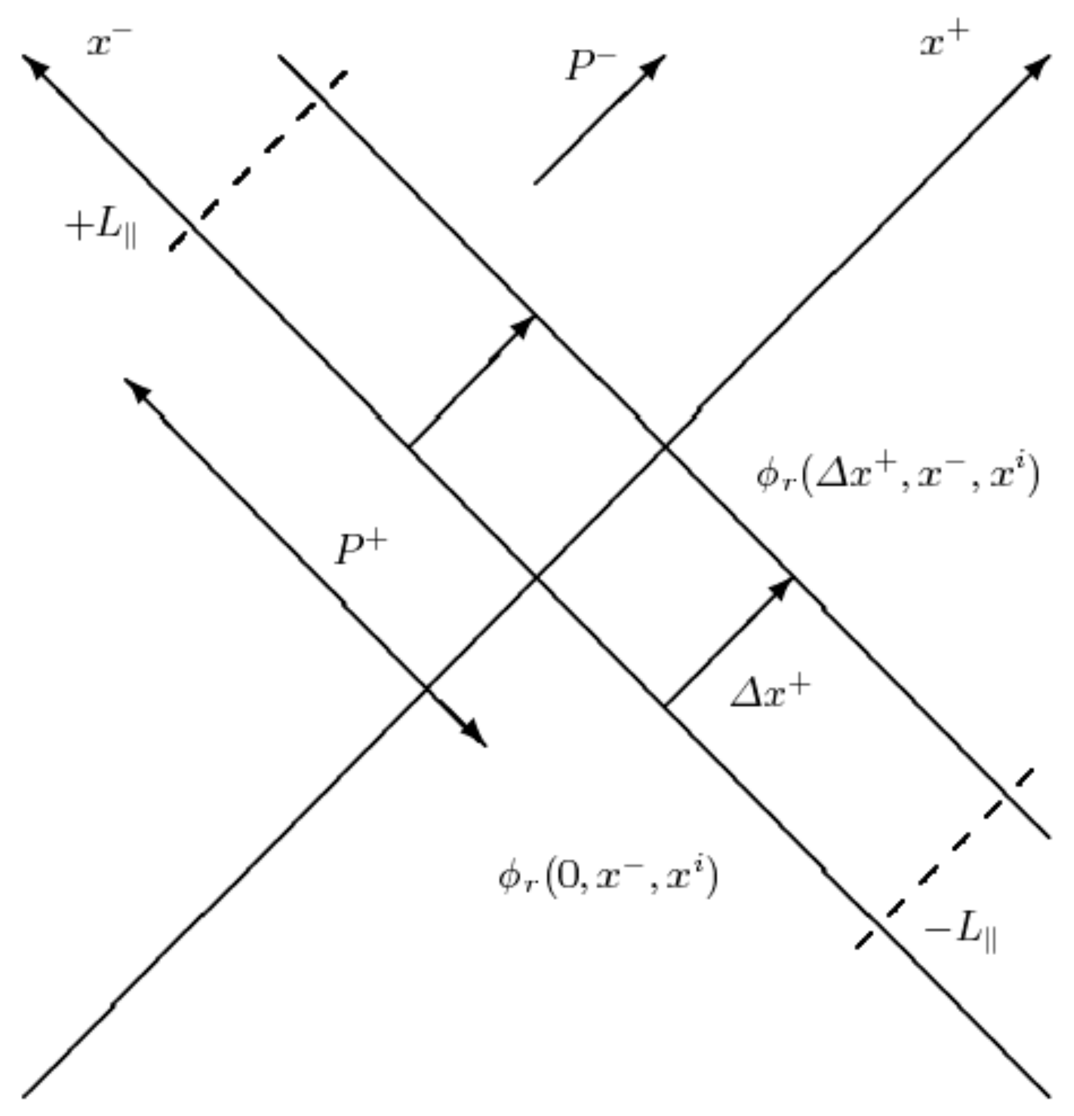
H. Honkanen, P. Maris, J. P. Vary and S. J. Brodsky,
"Electron in a transverse harmonic cavity",
Phys. Rev. Lett. 106, 061603 (2011); arXiv: 1008.0068

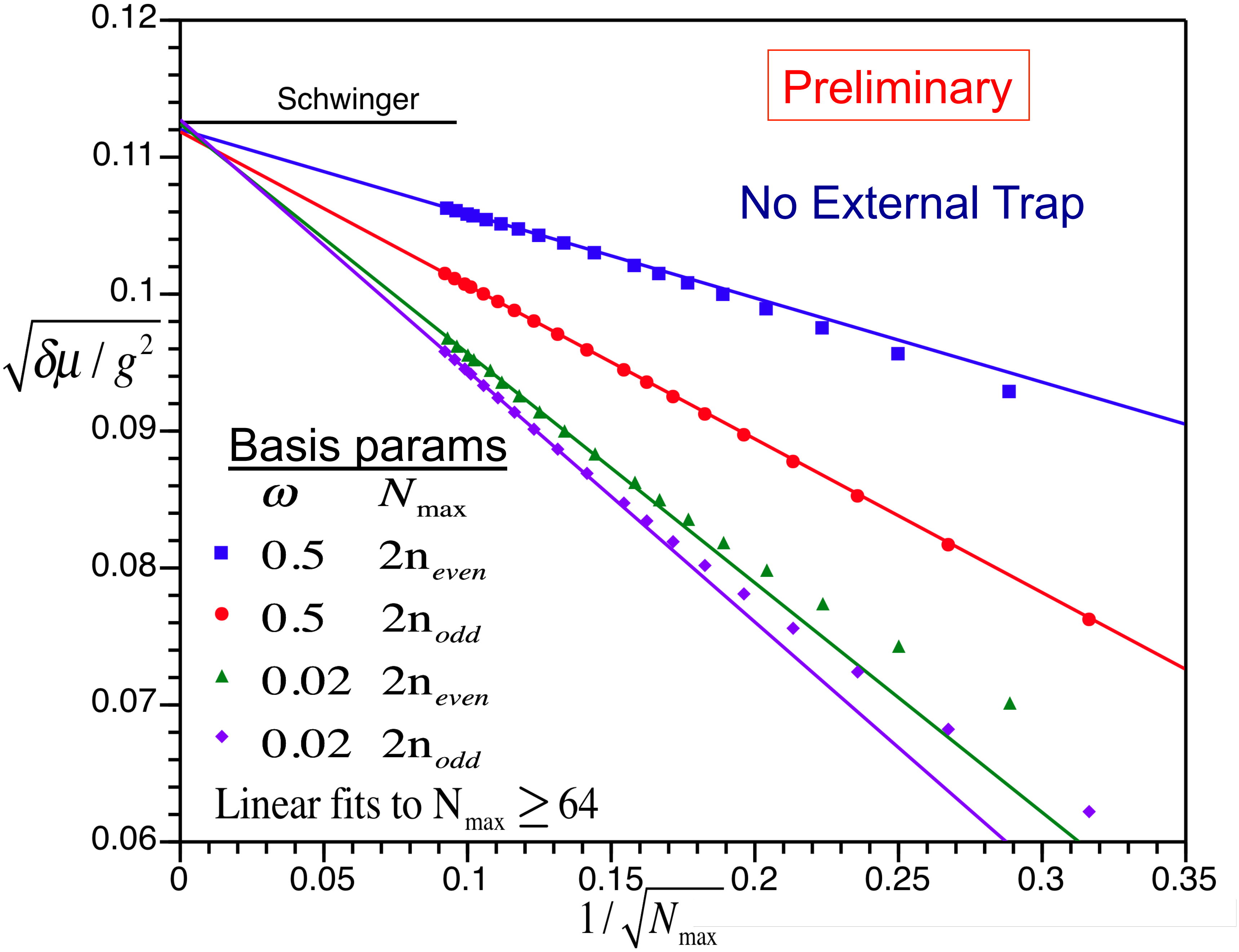
Light cone coordinates and generators

$$M^2 = P^0P_0 - P^1P_1 = (P^0 - P^1)(P_0 + P_1) = P^+P^- = KE$$

Equal time







X. Zhao, H. Honkanen, P. Maris, J.P. Vary, S.J. Brodsky, in preparation

Observation

Ab initio nuclear physics maximizes predictive power
& represents a theoretical and computational physics challenge

Key issues

How to achieve the full physics potential of *ab initio* theory?
Can theory and experiment work more closely
to define/solve fundamental physics problems?

Conclusions

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

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

Challenges

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

Collaborators – Nuclear Structure/Reactions

Nuclear Physics

ISU: Pieter Maris, Alina Negoita,
Chase Cockrell, Miles Aronnax
LLNL: Erich Ormand, Tom Luu, Eric Jurgenson
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, Heiko Hergert
WMU: Mihai Horoi
ANL: Harry Lee, Steve Pieper
LANL: Joe Carlson, Stefano Gandolfi
UA: Bruce Barrett, Sid Coon, Bira van Kolck,
Michael Kruse
LSU: Jerry Draayer, Tomas Dytrych,
Kristina Sviratcheva
UW: Martin Savage, Ionel Stetcu

International Collaborators

Canada: Petr Navratil
Russia: Andrey Shirokov,
Alexander Mazur
Sweden: Christian Forssen
Japan: Takashi Abe,
Takaharu Otsuka, Yutaka Utsuno
Noritaka Shimizu
Germany: Achim Schwenk,
Robert Roth, Javier Menendez,
students

Computer Science/Applied Math

Ames Lab: Masha Sosonkina,
Fang (Cherry) Liu, students
LBNL: Esmond Ng, Chao Yang,
Metin Aktulga
ANL: Stefan Wild
OSU: Umit Catalyurek

Collaborators – Quantum Field Theory

ISU: Heli Honkanen, Xingbo Zhao,
Pieter Maris, Paul Wiecki, Young Li
Stanford: Stan Brodsky

Germany: Hans-Juergen Pirner
Costa Rica: Guy de Teramond
India: Avaroth Harindranath

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 anomalous long lifetime of ^{14}C with chiral NN+NNN potentials