Ab initio nuclear structure – recent developments

"Nuclear Theory in the Supercomputing Era" Pacific National University

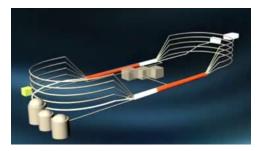


James P. Vary Iowa State University

June 18-22, 2012

Ab initio nuclear physics – fundamental ?'s





- 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?
- > Under what conditions do we need QCD to describe nuclear structure?













Blue Gene/P->Q



Hopper

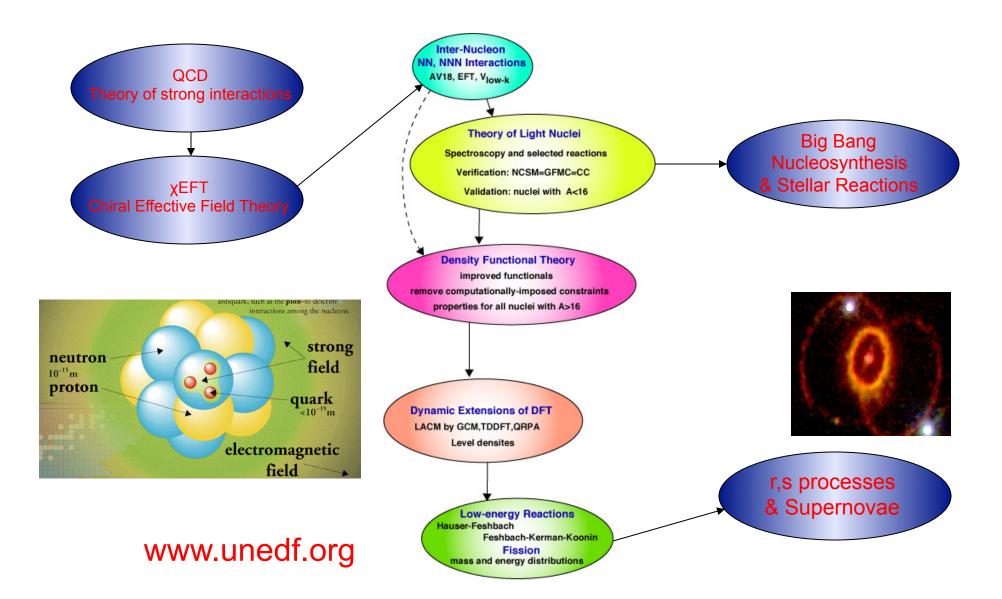


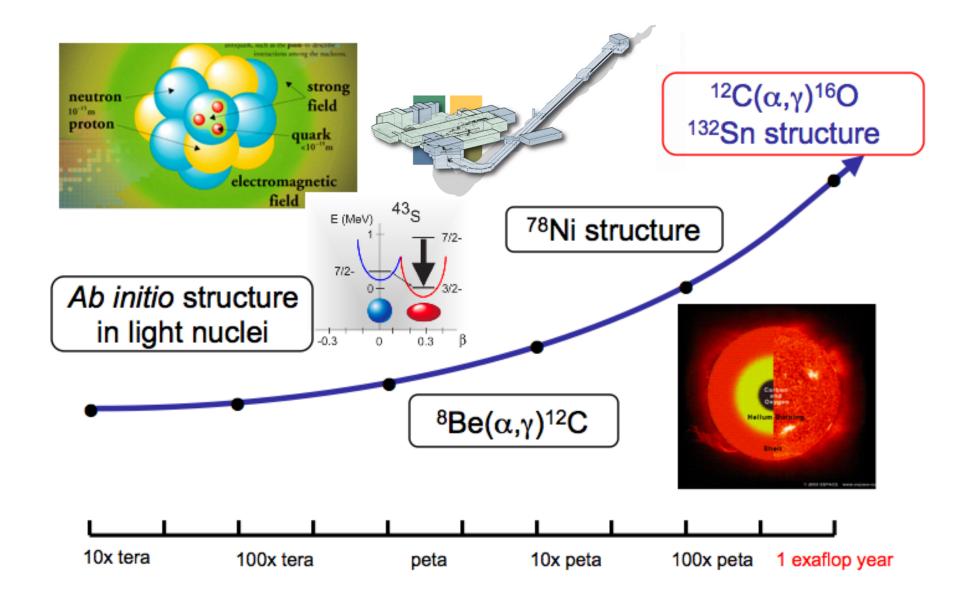
K-super. Blue Waters Lomonosov



UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional





The Nuclear Many-Body Problem

The many-body Schroedinger equation for bound states consists of $2^{A}\binom{A}{Z}$ 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 Shell Model (NCSM)
No Core Full Configuration (NCFC)

Cluster hierarchy in basis function space Coupled Cluster (CC)

Lattice + EFT approach (New)

Coming - Gorkov Green's Function, . . .

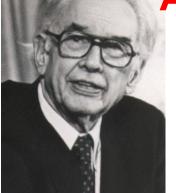
Comments

All work to preserve and exploit symmetries

Extensions of each to scattering/reactions are well-underway

They have different advantages and limitations

Atanasoff-Berry Computer (ABC)



John Vincent Atanasoff 1983 photo





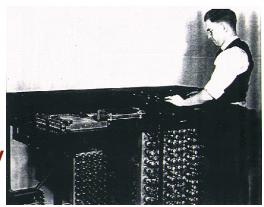
Clifford Berry 1962 photo

- •1939 Iowa State Physics Professor Atanasoff invents the electronic digital computer based on binary mathematics with stored program and data along with punch card input. Atanasoff and graduate student Clifford Berry construct the ABC and use ABC to solve simultaneous linear equations
- 1997 Replica completed and demonstrated in public

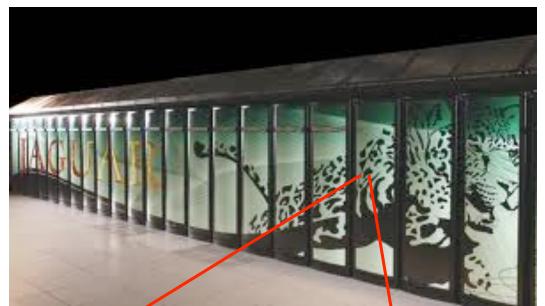


1990 - Atanasoff awarded the National Medal of Technology by President George W. Bush

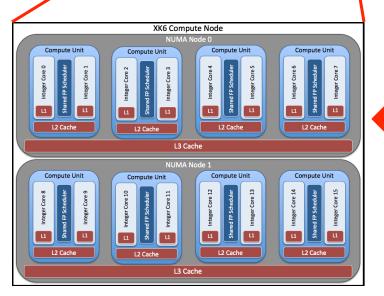
1942 photo of Clifford Berry and the ABC



"Leadership Class" Computational Resources







16 "cores" on one compute "node"

Total: 300,000 cores at present

Titan will have 1GPU/node

& INCITE Award 55M cpu-hrs/yr

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 $\lambda < 10^{19} \text{ GeV/c}$

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 $\lambda \sim 300 \text{ MeV/c} (1.5 \text{ fm}^{-1})$

"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

OLS: Okubo-Lee-Suzuki

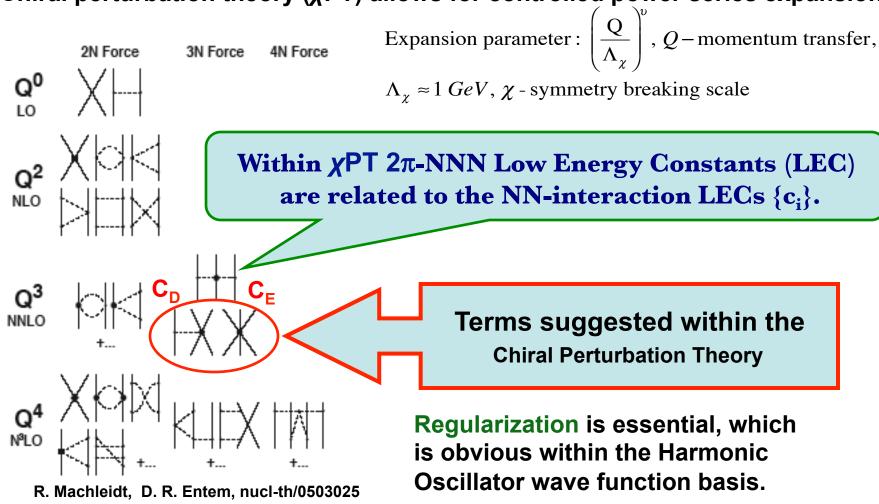
Vlowk: V with low k scale limit

UCOM: Unitary Correlation Operator Method

and there are more!

Effective Nucleon Interaction (Chiral Perturbation Theory)

Chiral perturbation theory (χ PT) allows for controlled power series expansion



No Core Shell Model A large sparse matrix eigenvalue problem

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

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

$$|\Psi_i\rangle = \sum_{n=0}^{\infty} A_n^i |\Phi_n\rangle$$
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 bookkeepping of anti-symmetrization)
- Diagonalize this sparse many-body H in its "m-scheme" basis where $[\alpha = (n,l,j,m_i,\tau_z)]$

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

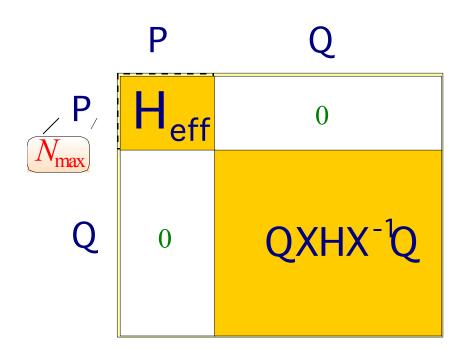
 $n = 1, 2, ..., 10^{10} \text{ or more!}$

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 Okubo-Lee-Suzuki renormalization scheme



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

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

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

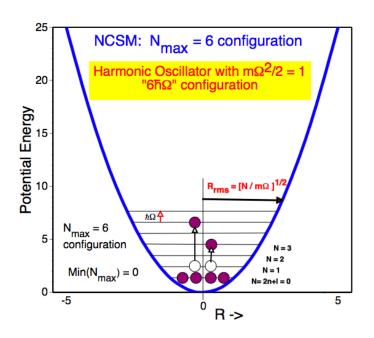
$$H_{\rm eff} = PXHX^{-1}P$$



- 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 $P: H^{(n)}_{eff} \rightarrow H_{eff}$



model space dimension

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

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

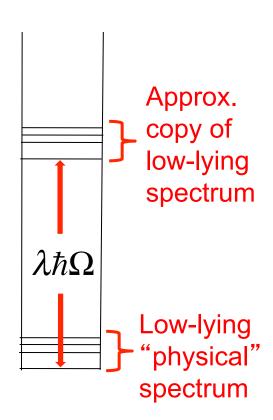
$$H_{eff}(N_{\text{max}},\hbar\Omega) \equiv P[T_{rel} + V^{a}(N_{\text{max}},\hbar\Omega)]P$$

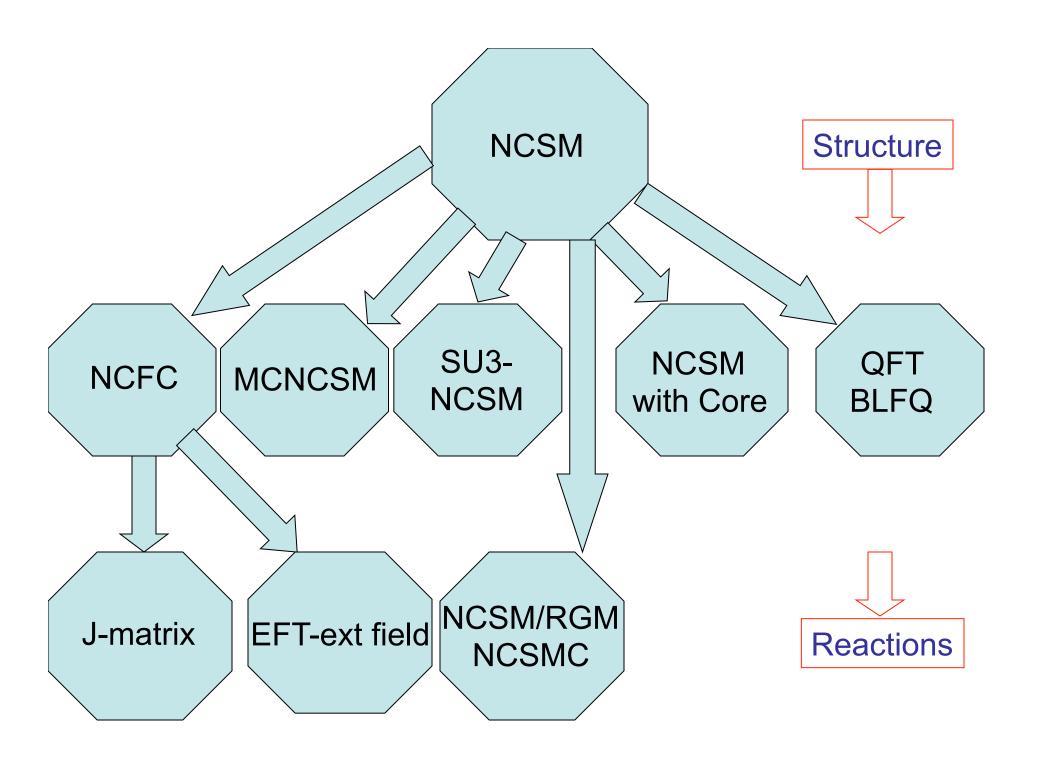
$$H = H_{eff}(N_{\text{max}}, \hbar\Omega) + \lambda H_{cm}$$

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

$$\lambda \sim 10$$
 suffices

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





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

P. Navrátil, V. G. Gueorguiev, 1,* J. P. Vary, 1,2 W. E. Ormand, and A. Nogga³

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"

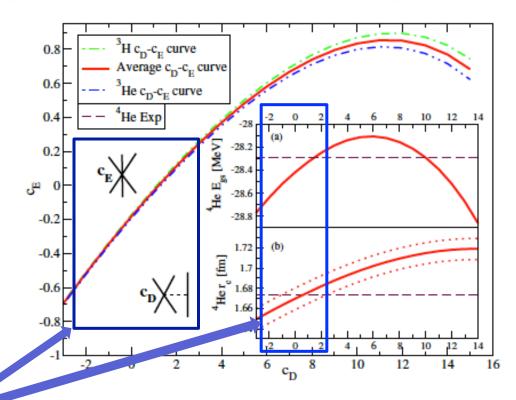
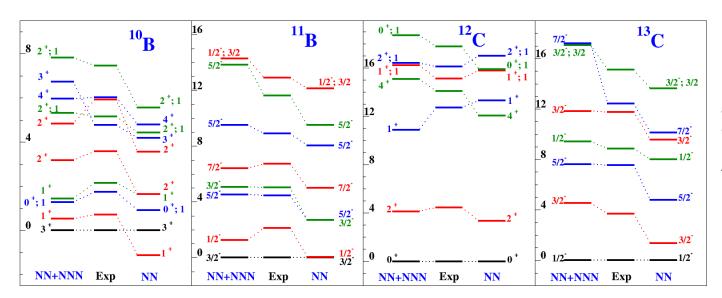


FIG. 1 (color online). Relations between c_D and c_E for which the binding energy of $^3\mathrm{H}$ (8.482 MeV) and $^3\mathrm{He}$ (7.718 MeV) are reproduced. (a) $^4\mathrm{He}$ ground-state energy along the averaged curve. (b) $^4\mathrm{He}$ charge radius r_c along the averaged curve. Dotted lines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

ab initio NCSM with χ_{FFT} Interactions

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



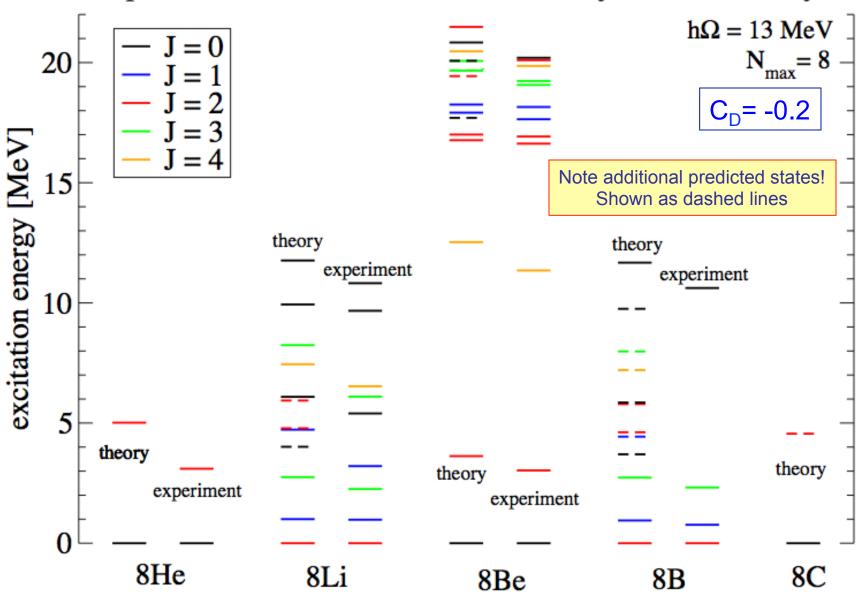
P. Navratil, V.G. Gueorguiev, J. P. Vary, W. E. Ormand and A. Nogga, PRL 99, 042501(2007); ArXiV: nucl-th 0701038.

$$c_{D} = -1$$

Extensions and work in progress

- Better determination of the NNN force itself, feedback to χ_{FFT} (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)

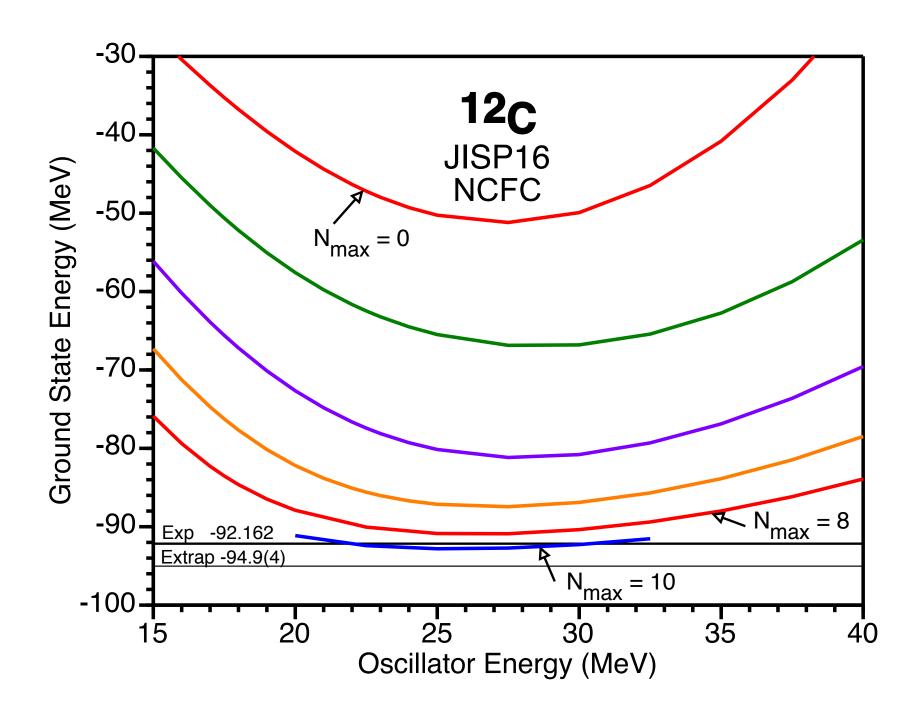
spectrum A=8 nuclei with N3LO 2-body + N2LO 3-body



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

Assessing Convergence

- \Box Independence of basis space parameters ($N_{\max},\hbar\Omega$)
- ☐ Each observable must be investigated separately
- ☐ Standard approach for gs energy (next slide)
- Newest approach (Sid Coon's talk at this meeting)



Convergence and Uncertainty Assessments: Recent Highlight

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

arXiv:1205.3230

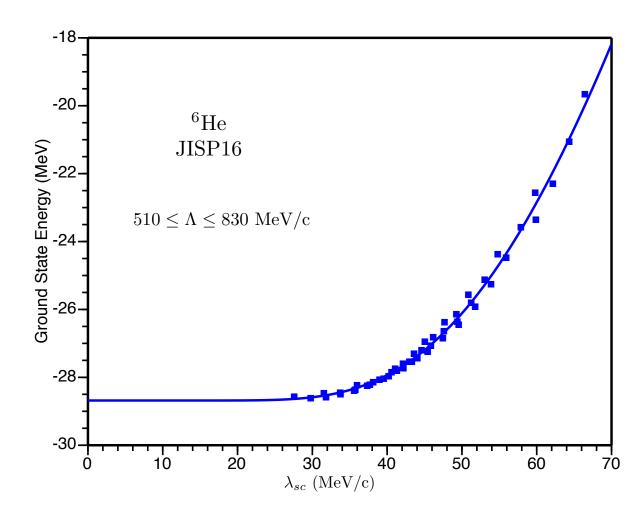
S. A. Coon^a, M. I. Avetian^a, M. K. G. Kruse^a, U. van Kolck^{a,b}, P. Maris^c, J. P. Vary^c

UV regulator:

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

IR regulator:

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



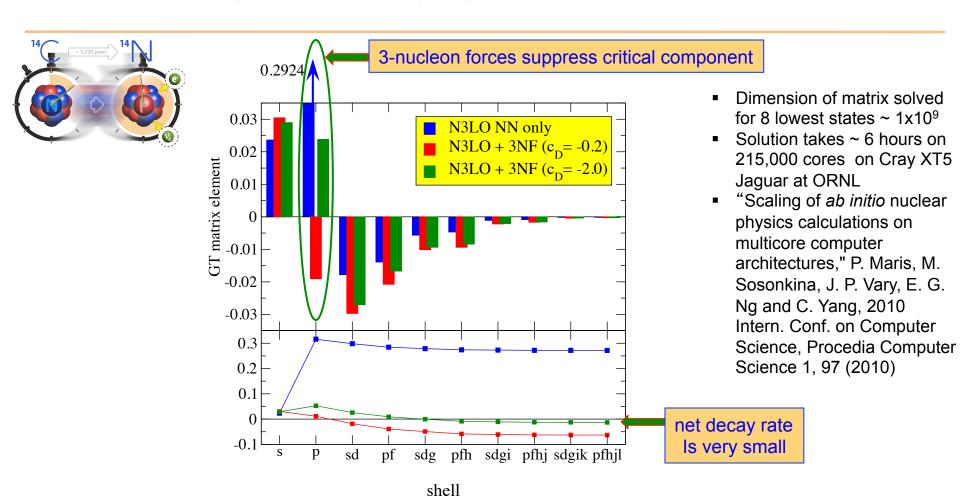


Origin of the Anomalous Long Lifetime of ¹⁴C

P. Maris, ¹ J. P. Vary, ¹ P. Navrátil, ^{2,3} W. E. Ormand, ^{3,4} H. Nam, ⁵ and D. J. Dean⁵



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



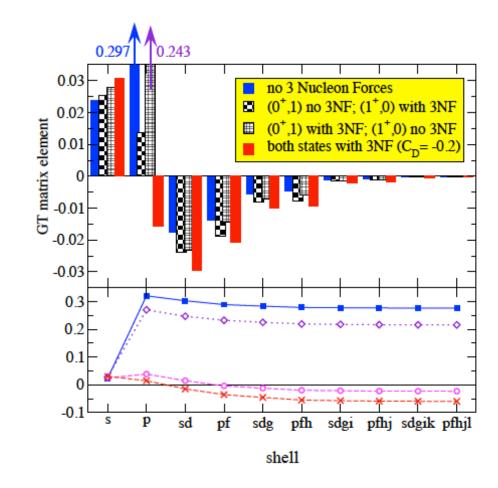


Figure 10. GT matrix element between the $(1^+,0)$ ground state and the lowest $(0^+,1)$ excited state of 14 N, using the $(1^+,0)$ wavefunction obtained with three-body forces, but the $(0^+,1)$ wavefunction obtained without three-body forces, and vice versa. For comparison, we also include the results with and without three-body forces for both wavefunctions.

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

SU(3) No Core Shell Model

Add symmetry-adapted many-body basis states
Preserve exactly the CM factorization
Talk by Thomas Dytrych at this meeting

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

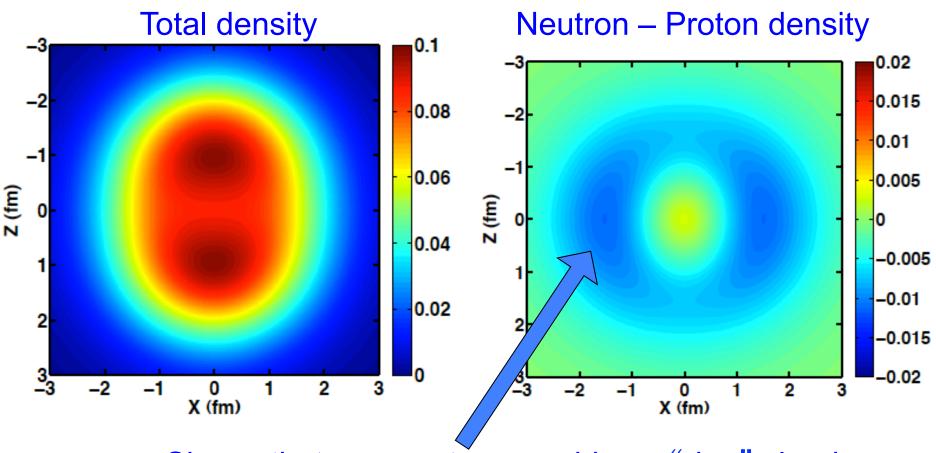
Talks by Yutaka Utsuno and Takashe Abe at this meeting

<u>Importance Truncated – NCSM</u>

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

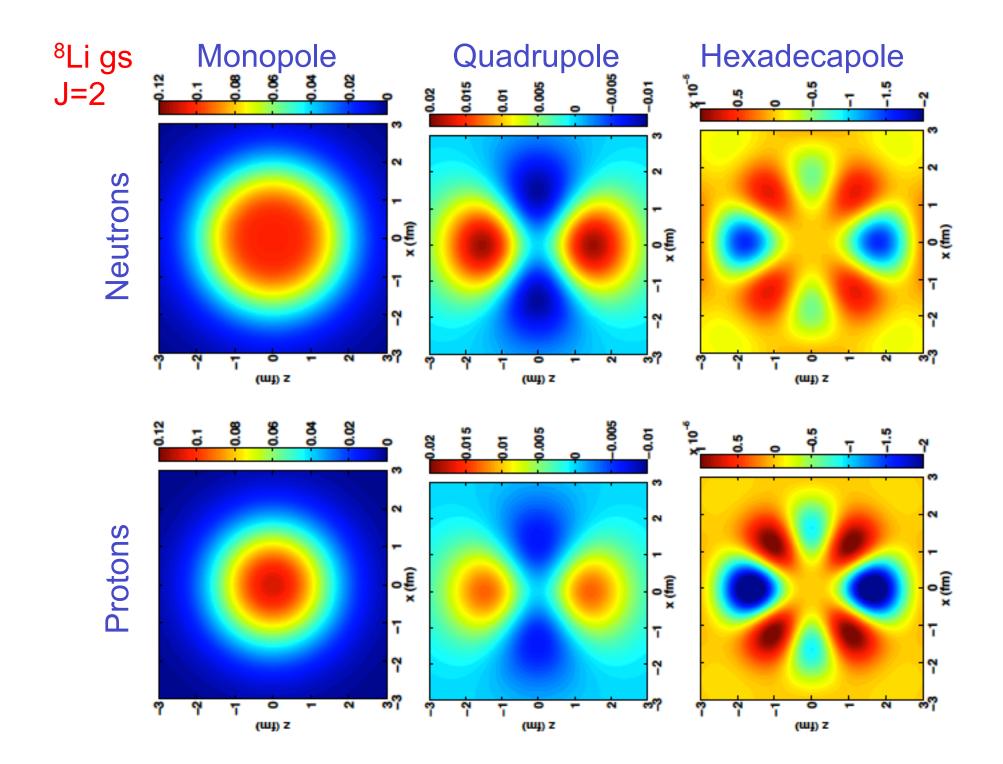
"Realistic" single-particle basis - Woods-Saxon example
Control the spurious CM motion with Lagrange multiplier term
A.Negoita, ISU PhD thesis
Alternative sp basis spaces – Mark Caprio collaboration

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

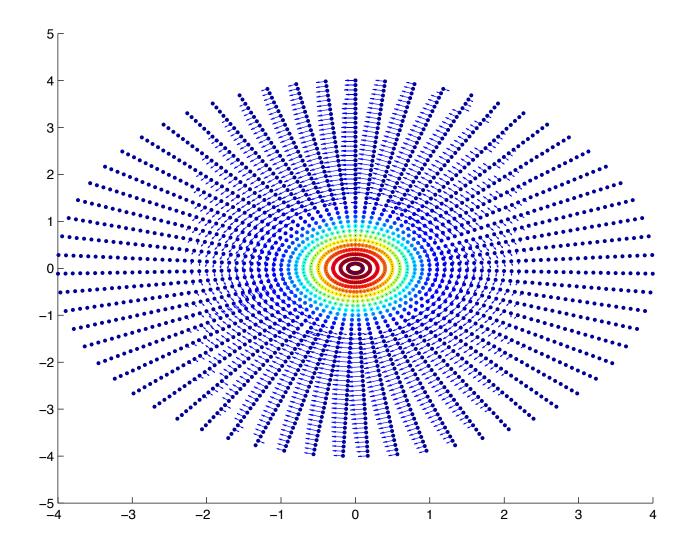


Shows that one neutron provides a "ring" cloud around two alpha clusters binding them together

C. Cockrell, J.P. Vary, P. Maris, ArXiv 1201.0724; C. Cockrell, PhD, Iowa State University

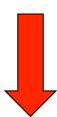


Wigner Distribution in 6LI – Demonstration/Preliminary



C. Cockrell, PhD Thesis, Iowa State 2012

Descriptive Science



Predictive Science

"Proton-Dripping Fluorine-14"

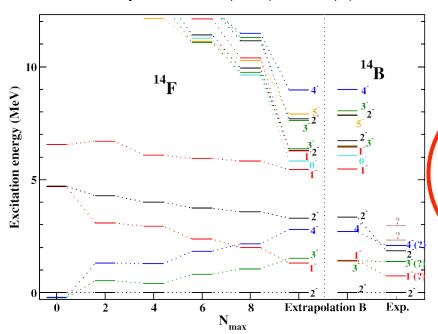
Objectives

 Apply ab initio microscopic nuclear theory's predictive power to major test case

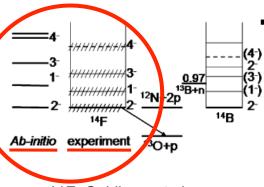
Impact

- 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 ~ 2x10⁹
- 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)



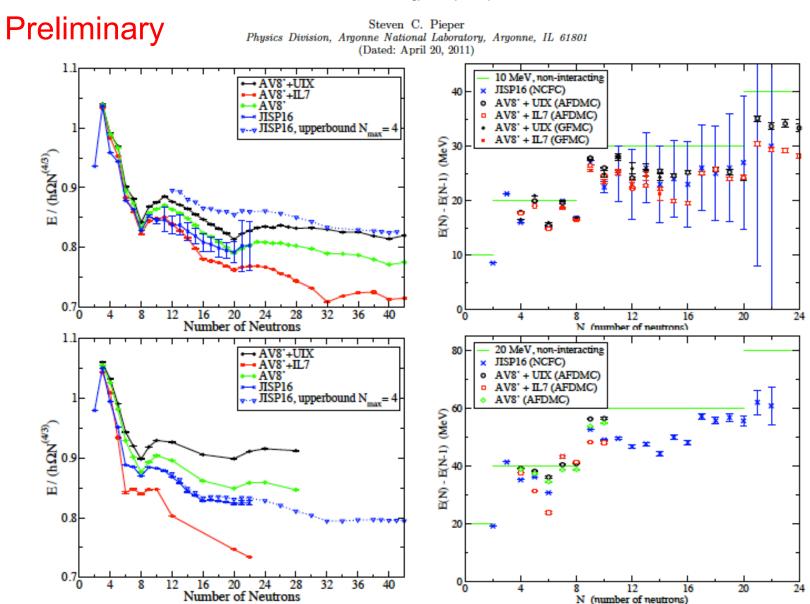




Properties of trapped neutrons interacting with realistic nuclear Hamiltonians

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



NCSM/RGM

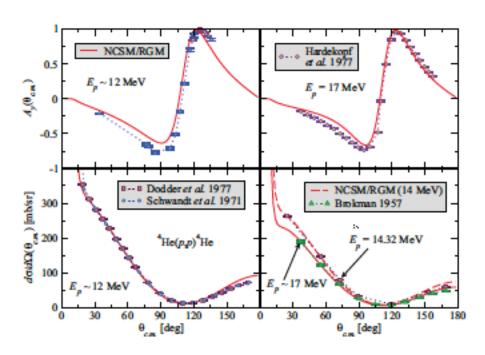


Figure 7. Calculated $p^{-4}He$ differential cross section (bottom panels) and analyzing power (top panels) for proton laboratory energies Ep = 12, 14.32 and 17 MeV compared to experimental data from Refs. [29, 30, 31, 32]. The SRG-N³LO NN potential with $\lambda = 2.02$ fm⁻¹ was used.

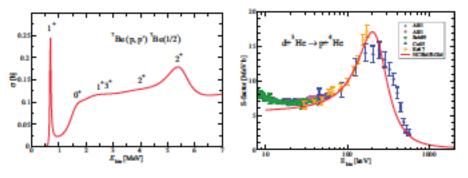


Figure 8. Calculated inelastic ${}^{7}Be(p,p'){}^{7}Be(1/2^{-})$ cross section with indicated positions of the P-wave resonances (left figure). Calculated S-factor of the ${}^{3}He(d,p){}^{4}He$ fusion reaction compared to experimental data (right figure). Energies are in the center of mass. The SRG-N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

J-matrix formalism:

scattering in the oscillator basis

$$T + V$$

$$\sum_{n'=0}^{N} H_{nn'}^{I} \langle n' | \lambda \rangle = E_{\lambda} \langle n | \lambda \rangle, \qquad n \leq N$$

$$G_{NN}(E) = -\sum_{\lambda=0}^{N} \frac{\langle N | \lambda \rangle^{2}}{E_{\lambda} - E}$$

$$S = \frac{C_{Nl}^{(-)}(q) - G_{NN}(E)T_{N,N+1}^{I}C_{N+1,l}^{(-)}(q)}{C_{Nl}^{(+)}(q) - G_{NN}(E)T_{N,N+1}^{I}C_{N+1,l}^{(+)}(q)}$$

n(p)+nucleus applications

Forward scattering J-matrix

- 1. Calculate E_{λ} and $\langle N | \lambda \rangle$ with NCSM
- 2. Solve for S-matrix and obtain phase shifts

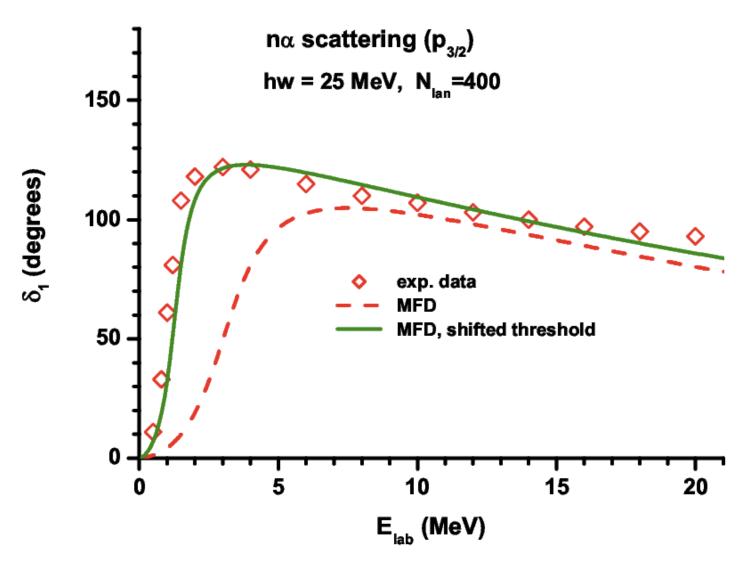
Inverse scattering J-matrix

- 1. Obtain phase shifts from scattering data
- 2. Solve for n(p)+nucleus potential, resonance params

Ί

A.M. Shirokov, A.I. Mazur, J.P. Vary, and E.A. Mazur, Phys. Rev. C. 79, 014610 (2009), arXiv:0806.4018; and references therein

nα scattering

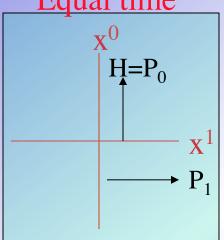


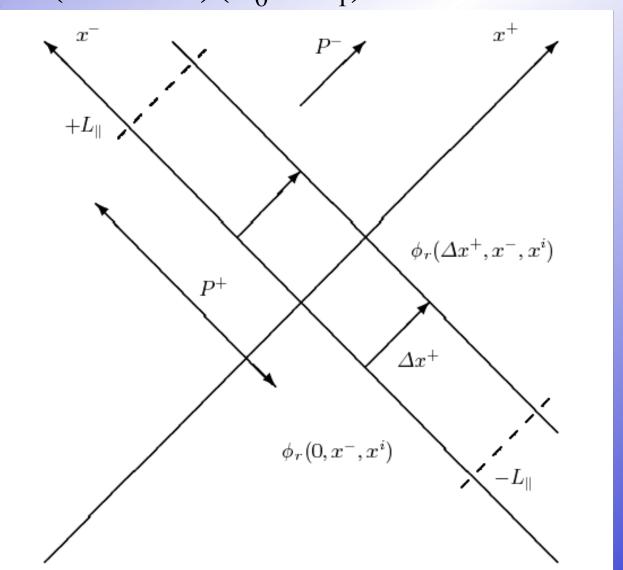
A. M. Shirokov, A. I. Mazur, J. P. Vary and E. A. Mazur, Phys. Rev. C. 79, 014610 (2009), arXiv 0806.4018

Light cone coordinates and generators

$$M^{2} = P^{0}P_{0} - P^{1}P_{1} = (P^{0} - P^{1})(P_{0} + P_{1}) = P^{+}P^{-} = KE$$

Equal time





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

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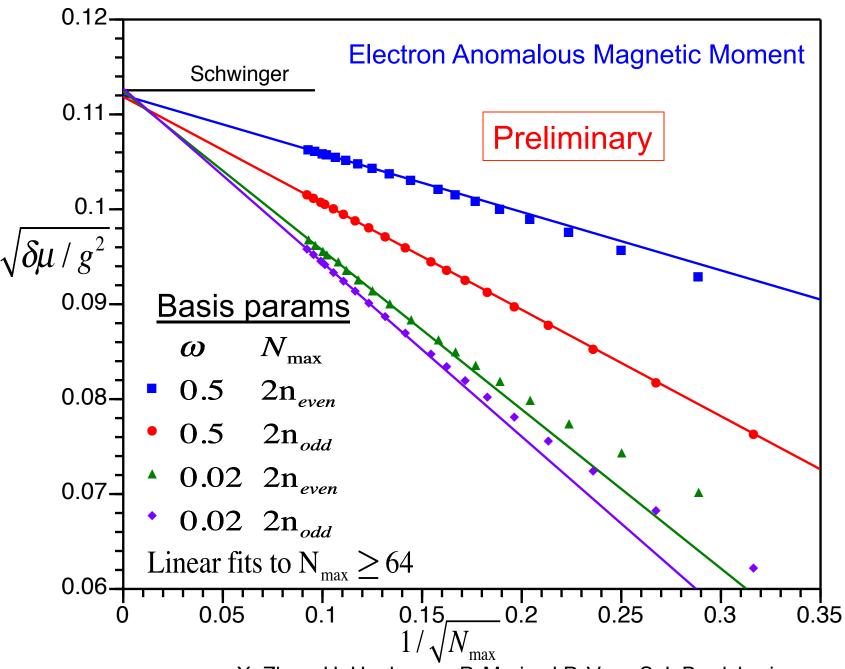
H. Honkanen, P. Maris, J. P. Vary and S. J. Brodsky, "Electron in a transverse harmonic cavity", Phys. Rev. Lett. 106, 061603 (2011); arXiv: 1008.0068

Basis Light Front Quantization (BLFQ) in brief

Derive LF Hamiltonian density from Lagrangian density Invoke canonical quantization

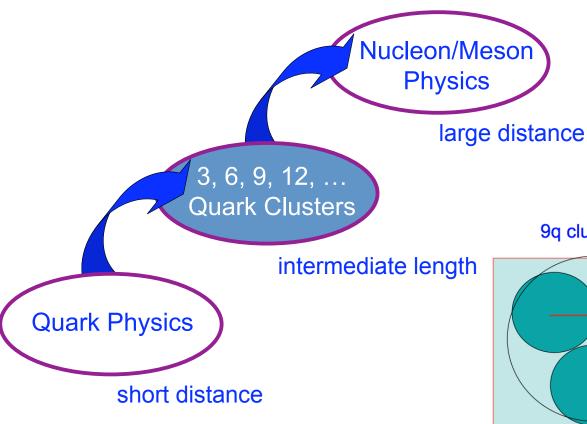
Evaluate H (kinetic term + vertices) in transverse 2D HO basis with longitudinal plane waves

Setup associated multi-parton Fock space basis
Diagonalize -> invariant mass spectra and LF amplitudes
Evaluate suite of observables and compare with experiment



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

Under what conditions do we require a quark-based description on nuclear structure? "Quark Percolation in Cold and Hot Nuclei"

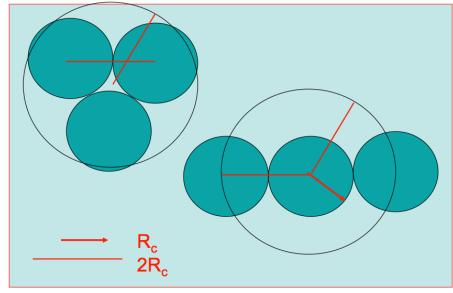


H.J. Pirner and J.P. Vary,

Phys. Rev. C. 84, 015201(2011);

arXiv: nucl-th/1008.4962

9q cluster at geometrical limits of formation



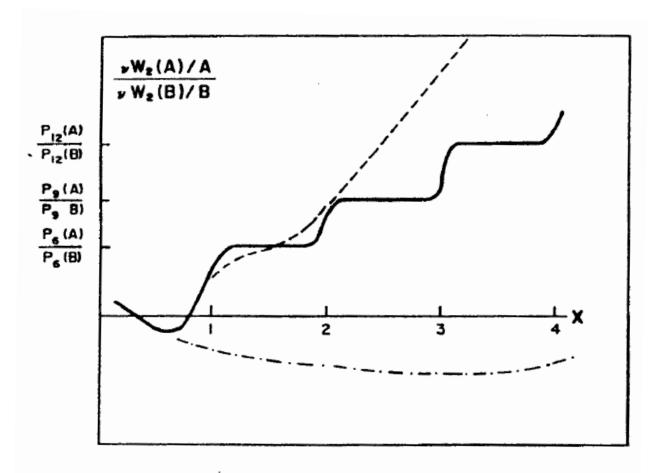


Fig. 2. Characteristic behaviour of the ratio of nuclear structure functions per nucleon for different models over a wide kinematic range of x. The QCM gives the solid curve. The dashed curve is due to the model of reference 22. The dashed-dot curve approximates the predictions of references 23 and 24.

J.P. Vary, Proc. VII Int'l Seminar on High Energy Physics Problems, "Quark Cluster Model of Nuclei and Lepton Scattering Results," Multiquark Interactions and Quantum Chromodynamics, V.V. Burov, Ed., Dubna #D-1, 2-84-599 (1984) 186 [staircase function for x > 1]

See also: Proceedings of HUGS at CEBAF1992, & many conf. proceedings

New Measurements of High-Momentum Nucleons and Short-Range Structures in Nuclei

N. Fomin, ^{1,2,3} J. Arrington, ⁴ R. Asaturyan, ^{5,*} F. Benmokhtar, ⁶ W. Boeglin, ⁷ P. Bosted, ⁸ A. Bruell, ⁸ M. H. S. Bukhari, ⁹ M. E. Christy, ⁸ E. Chudakov, ⁸ B. Clasie, ¹⁰ S. H. Connell, ¹¹ M. M. Dalton, ³ A. Daniel, ⁹ D. B. Day, ³ D. Dutta, ^{12,13} R. Ent, ⁸ L. El Fassi, ⁴ H. Fenker, ⁸ B. W. Filippone, ¹⁴ K. Garrow, ¹⁵ D. Gaskell, ⁸ C. Hill, ³ R. J. Holt, ⁴ T. Horn, ^{6,8,16} M. K. Jones, ⁸ J. Jourdan, ¹⁷ N. Kalantarians, ⁹ C. E. Keppel, ^{8,18} D. Kiselev, ¹⁷ M. Kotulla, ¹⁷ R. Lindgren, ³ A. F. Lung, ⁸ S. Malace, ¹⁸ P. Markowitz, ⁷ P. McKee, ³ D. G. Meekins, ⁸ H. Mkrtchyan, ⁵ T. Navasardyan, ⁵ G. Niculescu, ¹⁹ A. K. Opper, ²⁰ C. Perdrisat, ²¹ D. H. Potterveld, ⁴ V. Punjabi, ²² X. Qian, ¹³ P. E. Reimer, ⁴ J. Roche, ^{20,8} V. M. Rodriguez, ⁹ O. Rondon, ³ E. Schulte, ⁴ J. Seely, ¹⁰ E. Segbefia, ¹⁸ K. Slifer, ³ G. R. Smith, ⁸ P. Solvignon, ⁸ V. Tadevosyan, ⁵ S. Tajima, ³ L. Tang, ^{8,18} G. Testa, ¹⁷ R. Trojer, ¹⁷ V. Tvaskis, ¹⁸ W. F. Vulcan, ⁸ C. Wasko, ³ F. R. Wesselmann, ²² S. A. Wood, ⁸ J. Wright, ³ and X. Zheng^{3,4}

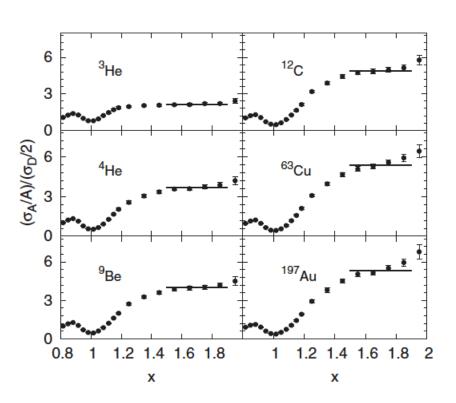


FIG. 2. Pernucleon cross section ratios vs x at $\theta_e = 18^{\circ}$.

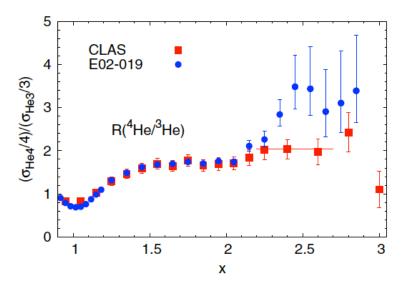
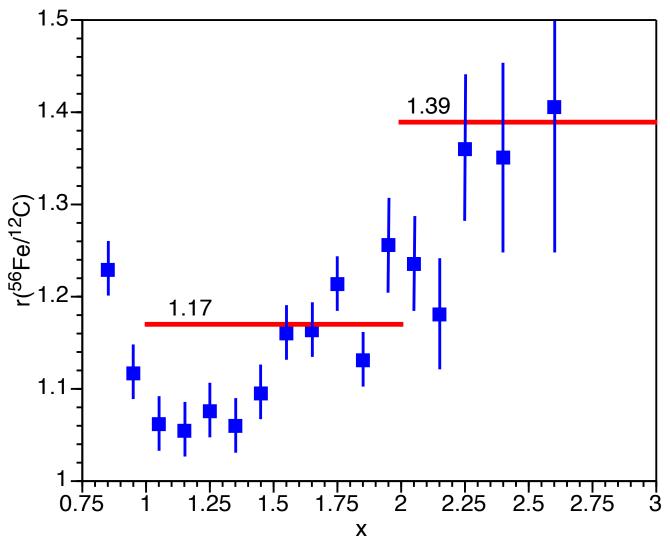


FIG. 3 (color online). The ${}^4{\rm He}/{}^3{\rm He}$ ratios from E02-019 ($Q^2 \approx 2.9~{\rm GeV^2}$) and CLAS ($\langle Q^2 \rangle \approx 1.6~{\rm GeV^2}$); errors are combined statistical and systematic uncertainties. For x > 2.2, the uncertainties in the ${}^3{\rm He}$ cross section are large enough that a one-sigma variation of these results yields an asymmetric error band in the ratio. The error bars shown for this region represent the central 68% confidence level region.

Comparison between Quark-Cluster Model and JLAB data



Data: K.S. Egiyan, et al., Phys. Rev. Lett. **96**, 082501 (2006)

Theory: H.J. Pirner and J.P. Vary, Phys. Rev. Lett. **46**, 1376 (1981)
and Phys. Rev. C **84**, 015201 (2011); nucl-th/1008.4962;
M. Sato, S.A. Coon, H.J. Pirner and J.P. Vary, Phys. Rev. C **33**, 1062 (1986)

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 6Li
- ➤ Established need for NNN potentials to explain neutrino -12C 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 ¹⁰B by including chiral NNN potentials
- ➤ Successful prediction of low-lying ¹⁴F spectrum (resonances) before experiment
- > Developed/applied methods to extract phase shifts (J-matrix, external trap)
- ➤ Explained the anomalous long lifetime of ¹⁴C with chiral NN+NNN potentials
- > Solved systems of trapped neutrons for improved density functionals in isospin extremes

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

Applications underway to Light Front QCD and strong time-dependent QED

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

Nuclear Physics Recent Collaborators International

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

Notre Dame: Mark Caprio

ANL: Harry Lee, Steve Pieper

LANL: Joe Carlson, Stefano Gandolfi

UA: Bruce Barrett, Sid Coon, Bira van Kolck,

Michael Kruse, Matthew Avetian

LSU: Jerry Draayer, Tomas Dytrych,

Kristina Sviratcheva, Chairul Bahri

UW: Martin Savage, Ionel Stetcu

Canada: Petr Navratil

Russia: Andrey Shirokov,

Alexander Mazur, Eugene Mazur,

Sergey Zaytsev, Vasily Kulikov

Sweden: Christian Forssen

Japan: Takashi Abe,

Takaharu Otsuka, Yutaka Utsuno

Noritaka Shimizu

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Robert Roth, Javier Menendez,

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OSU: Umit Catalyurek, Eric Saule

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Asmita Mukheriee