Ab initio Nuclear Theory Recent progress & future prospects

> James P. Vary Iowa State University

November 24, 2010

NN Interaction & Nuclear Many-Body Problem TIFR - Mumbai

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

Application drivers for increased computational power

- Frontiers of theoretical physics
- Simulations/Data Analysis for large experiments
- Downscaling of climate modeling
- Proteomics Gene therapies
- Search engines dynamic knowledge systems
- Economic modeling and market forecasting
- Pharmaceutical development
- Stockpile stewardship









Some Frontiers in Theoretical Physics: Quantum Many-Body and Mesoscopic Science -Sharing methods and computational resources

- Cold trapped atoms (talks at this workshop)
- Quantum dots (next slide)
- Quantum chemistry of molecules (spectra and reactions)
- Condensed matter physics (graphene, fullerine, . . .)
- Atomic physics (spectra and reactions)
- Nuclear physics (workshop talks, main focus of this talk)
- Quantum field theory (later in this talk)

Nuclei and Quantum Dots



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?











Bridging the nuclear physics scales



Adapted from D. Dean, JUSTIPEN Meeting, 2009

Applications in astrophysics, defense, energy, and medicine

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 $^{12}C(\alpha,\gamma)^{16}O$





Testing the doubly magic character of tin-132

Adding an extra neutron to a nucleus with magic numbers of both neutrons and protons, and watching how it settles in, tests the shell model and can help elucidate the creation of heavy elements in supernovae.



Doubly magic shell game

Based on: K.L. Jones, et al., *Nature* **465**, 454 (2010) P. Cottle, *Nature* **465**, 430 (2010)



Figure 2. Doubly magic nuclides tin-132 and lead-208 clearly manifest special properties when compared, from archival data, with lighter isotopes that also have even neutron numbers *N*. **(a)** The energy of the first electricquadrupole excitation peaks dramatically at N_{magic} (82 for Sn, 126 for Pb). **(b)** The energy cost of removing a neutron pair falls abruptly after N_{magic} . (Adapted from ref. 1.)



Figure 4. Valence states of the extra tin-133 neutron. For each of the valence levels observed in the Oak Ridge experiment, schematically shown above the doubly magic ¹³²Sn core, the best-fit quantum state is given (left) together with its spectroscopic factor *S* (right), a measure of spectral purity. In the spectroscopic notation, *p* and *f* denote, respectively, orbital angular momenta 1 and 3. If the best-fit state is pure, with no admixture of other quantum states due to core excitations, *S* = 1. (Adapted from ref. 1.)



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 $\lambda \sim 600 \text{ MeV/c} (3.0 \text{ fm}^{-1})$

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 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 (χ PT) allows for controlled power series expansion



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

- 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
- Matches well with results of chiral NN + NNN interactions
- 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

The Nuclear Many-Body Problem

The many-body Schroedinger equation for bound states consists of $2\binom{A}{Z}$ coupled second-order differential equations in 3A coordinates using strong (NN & NNN) and electromagnetic interactions.

Successful ab initio quantum many-body approaches (A > 6)

Stochastic approach in coordinate space Greens Function Monte Carlo (**GFMC**)

Hamiltonian matrix in basis function space No Core Shell Model (**NCSM**) No Core Full Configuration (**NCFC**)

Cluster hierarchy in basis function space Coupled Cluster (**CC**)

Comments

All work to preserve and exploit symmetries Extensions of each to scattering/reactions are well-underway They have different advantages and limitations



No Core Shell Model

A large sparse matrix eigenvalue problem

$$H = T_{rel} + V_{NN} + V_{3N} + \bullet \bullet$$
$$H |\Psi_i\rangle = E_i |\Psi_i\rangle$$
$$|\Psi_i\rangle = \sum_{n=0}^{\infty} A_n^i |\Phi_n\rangle$$
Diagonalize {\lap\leftarrow \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 $[\alpha = (n,l,j,m_i,\tau_z)]$

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

n = 1,2,...,10¹⁰ 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



$$H: E_{1}, E_{2}, E_{3}, \dots E_{d_{P}}, \dots E_{\infty}$$
$$H_{eff}: E_{1}, E_{2}, E_{3}, \dots E_{d_{P}}$$
$$QXHX^{-1}P = 0$$
$$M_{eff} = PXHX^{-1}P$$
$$unitary X = exp[-arctan h(\omega^{+} - \omega)]$$

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



"Walkthrough" of HO wavefunctions nlm = 221 & superposition: 111+331







P. Maris, A. Shirokov and J.P. Vary, Phys. Rev. C81, 021301 (R) (2010). ArXiv 0911.2281

NCSM with Chiral NN (N3LO) + NNN (N2LO, C_D =-0.2)



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

Beryllium isotopes



updated from Vary, Maris, Ng, Yang, Sosonkina, arXiv:0907.0209 [nucl-th],

J. Phys. Conf. Ser. 180, 012083 (2009)

- Exploring physics near the neutron drip line in progress
- Un-natural parity states systematically underbound with JISP16
- Similar results for He- and Li-isotopes



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)

v-¹²C cross section and the 0⁺ -> 1⁺ 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

Will be updated with $N_{max} = 8$ results

Non-local NN interaction from inverse scattering also successful



How good is *ab initio* theory for predicting large scale collective motion?

Quantum rotator





¹²C - At the heart of matter

The first excited 0+ state of ¹²C, the "Hoyle state", is the key state of ¹²C 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 ¹²C 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 achievable with petascale within 1-2 years



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



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 	Change to physically relevant basis H.O. basis



American Physical Society physical Log in | Create Account (what's this?) RSS Feeds | Email Alerts

Phys. Rev. Lett. 104, 182501 (2010) [4 pages]

Ab Initio Computation of the ¹⁷F Proton Halo State and Resonances in A=17 Nuclei

G. Hagen¹, T. Papenbrock^{2,1}, and M. Hjorth-Jensen³

¹Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

²Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA

³Department of Physics and Center of Mathematics for Applications, University of Oslo, N-0316 Oslo, Norway

Received 9 March 2010; published 4 May 2010

	¹⁷ O			¹⁷ F		
	$1/2^{+}$	$5/2^{+}$	E_{so}	$1/2^{+}$	$5/2^{+}$	E_{so}
GHF	-2.8	-3.2	4.3	-0.082	0.11	3.7
Exp.	-3.272	-4.143	5.084	-0.105	-0.600	5.000

TABLE I: Single-particle energies of the $1/2^+$ and $5/2^+$ states, and the spin-orbit splitting $E_{so}(d_{3/2}-d_{5/2})$ (in units of MeV) in ¹⁷O and ¹⁷F calculated in a Berggren (Gamow) basis (GHF), and the comparison to experiment [31].

	¹⁷ O 3/2 ⁺		$^{17}F 3/2^+$	
	$E_{\rm sp}$	Г	$E_{\rm sp}$	Г
This work	1.1	0.014	3.9	1.0
Experiment	0.942	0.096	4.399	1.530

TABLE II: Computed $3/2^+$ single-particle resonance energies in ¹⁷O and ¹⁷F compared to data [31]. The real part $E_{\rm sp} =$ Re[E], and the width $\Gamma = 2 \text{Im}[E]$ are given in units of MeV.

Descriptive Science

Predictive Science



First observation of ¹⁴F

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

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

Ab initio Nuclear Structure Ab initio Nuclear Reactions

Ab initio NCSM/RGM: nucleon-⁴He scattering

 The N-⁴He potential is calculated microscopically from the manybody realistic Hamiltonian and the NCSM eigenstates of the ⁴He

$$4He \int \hat{\mathcal{A}}(H-E)\hat{\mathcal{A}} = W_{VV'}(r,r')$$

 Solving the non-local integro-differential coupled-channel equations for the N-⁴He relative motion: phase shifts, cross sections, polarization observables

calculated microscopically from the many-



Navratil



J-matrix formalism: scattering in the oscillator basis



2. Solve for n(p)+nucleus potential, resonance params

and references therein

$n\alpha$ 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



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



Observation

Ab initio nuclear physics shares methods and computational resources with other fields of physics.

Key Challenge

How to capitalize on the predictive power and 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

Collaborators – Nuclear Structure/Reactions

Nuclear Physics

ISU: Pieter Maris, James Vary, students LLNL: Petr Navratil, 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, students/postdocs UW: Martin Savage TRIUMF/GSI: Achim Schwenk

International Collaborators

Russia: Andrey Shirokov, Alexander Mazur Sweden: Christian Forssen, Japan: Takashi Abe, Takaharu Otsuka, Yutaka Utsuno Noritaka Shimizu

Computer Science/Applied Math

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

Collaborators – Quantum Field Theory

ISU: Heli Honkanen, Pieter Maris Stanford: Stan Brodsky Heidelberg: Hans-Juergen Pirner 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 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)