From QCD to ab initio nuclear structure with point nucleons and back again

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Ab initio nuclear physics – fundamental ?’s

- 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?
- Under what conditions do we need QCD to describe nuclear structure?
QCD
Theory of strong interactions

χEFT
Chiral Effective Field Theory

Inter-Nucleon
NN, NNN interactions
AV18, EFT, \( V_{\text{low-k}} \)

Theory of Light Nuclei
Spectroscopy and selected reactions
Verification: NCSM=GFM\( \rightarrow \)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 densities

Low-energy Reactions
\( \text{Hauser-Feshbach} \)
\( \text{Feshbach-Kerman-Koonin} \)
\( \text{Fission} \)
mass and energy distributions

r,s processes
\& Supernovae

www.unedf.org
The Nuclear Many-Body Problem

The many-body Schrödinger equation for bound states consists of $2^A \binom{A}{2}$ 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
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
\( \lambda \sim 600 \text{ MeV/c (3.0 fm}^{-1}) \)

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

“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.

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**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!
Chiral perturbation theory ($\chi$PT) allows for controlled power series expansion

Expansion parameter: \( \left( \frac{Q}{\Lambda_\chi} \right)^n \), \( Q \) – momentum transfer,
\( \Lambda_\chi \approx 1 \text{ GeV} \), \( \chi \) - symmetry breaking scale

Within $\chi$PT $2\pi$-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

\[ H = T_{rel} + V_{NN} + V_{3N} + \cdots \]
\[ H|\Psi_i\rangle = E_i|\Psi_i\rangle \]
\[ |\Psi_i\rangle = \sum_{n=0}^{\infty} A_n^i |\Phi_n\rangle \]
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, \( \alpha, \beta, \ldots \)
- 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 \( [\alpha = (n,l,j,m_j,\tau_z)] \)
\[ |\Phi_n\rangle = [a_\alpha^+ \cdots a_\zeta^+]_n |0\rangle \]
\( n = 1, 2, \ldots, 10^{10} \) 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 renormalization scheme

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

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

\[ H = H_{\text{eff}} \left( N_{\text{max}}, \hbar \Omega \right) + \lambda H_{cm} \]

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

\[ \lambda \sim 10 \text{ suffices} \]

Along with the \( N_{\text{max}} \) 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 translationally invariant wavefunction.
Strong correlation between $c_D$ and $c_E$ for experimental properties of $A = 3$ & 4

=> Retain this correlation in applications to other systems

Range favored by various analyses & values are “natural”
**ab initio NCSM with $\chi_{EFT}$ Interactions**

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

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**Extensions and work in progress**

- Better determination of the NNN force itself, feedback to $\chi_{EFT}$ (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)

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

$C_D = -1$
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
- Solves the puzzle of the long but useful lifetime of $^{14}\text{C}$
- Establishes a major role for strong 3-nucleon forces in nuclei
- Strengthens foundation for guiding DOE-supported experiments

- Dimension of matrix solved for 8 lowest states $\sim 1\times10^9$
- Solution takes $\sim 6$ hours on 215,000 cores on Cray XT5 Jaguar at ORNL
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 \textit{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
$^7$Li – effect of removing spurious CM motion

Chase Cockrell, ISU PhD student
9Be Translationally invariant gs density
Full 3D densities = rotate around the vertical axis

Total density  Proton - Neutron density

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

Chase Cockrell, ISU PhD student
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

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**Experiment confirms our published predictions!**


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Dimension of matrix solved for 14 lowest states $\sim 2 \times 10^9$

Solution takes $\sim 2.5$ hours on 30,000 cores (Cray XT4 Jaguar at ORNL)

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”,
Light cone coordinates and generators

\[ M^2 = P^0 P_0 - P^1 P_1 = (P^0 - P^1)(P_0 + P_1) = P^+ P^- = KE \]
Electron Anomalous Magnetic Moment

$\sqrt{\delta \mu / g^2}$

Basis params

$\omega$ $N_{\text{max}}$

- 0.5 $2n_{\text{even}}$
- 0.5 $2n_{\text{odd}}$
- 0.02 $2n_{\text{even}}$
- 0.02 $2n_{\text{odd}}$

Linear fits to $N_{\text{max}} \geq 64$

Sample planned Applications for BLFQ

Strong pulsed laser fields – electron-positron pair creation

Quarkonia – structure & transitions - including exotics

Baryons – mass spectra, spin content,
   Generalized Parton Distributions (GPDs)
Under what conditions do we need quarks & gluons to describe nuclear structure?

1. Spin crisis in the proton
2. Proton RMS radius
3. DIS on nuclei – Bjorken $x > 1$
4. Nuclear Equation of State
5. $Q > 1 \text{ GeV/c}$
New Measurements of High-Momentum Nucleons and Short-Range Structures in Nuclei


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

FIG. 3 (color online). The $^4\text{He}/^3\text{He}$ ratios from E02-019 ($Q^2 \approx 2.9$ GeV$^2$) and CLAS ($Q^2 \approx 1.6$ GeV$^2$); errors are combined statistical and systematic uncertainties. For $x > 2.2$, the uncertainties in the $^3\text{He}$ 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.
DIS in the quark cluster model

\[
\frac{\nu}{\sigma_m} \frac{d^2 \sigma}{d\Omega dE'} = \nu W_2(\nu, Q^2) + \nu W_1(\nu, Q^2) \tan^2(\theta/2)
\]

\[

\nu W_2(\nu, Q^2) = \nu W_2^{in}(\nu, Q^2) + \nu W_2^{q_{-e1}}(\nu, Q^2)
\]

\[
\nu W_2^{in}(\nu, Q^2) = \sum_{\text{quarks}-j} e_j^2 \xi P(\xi)
\]

\[
P(\xi) = \sum_{\text{clusters}-i} p_i \bar{P}_i(\xi)
\]

\[
\bar{P}_i(\xi) = \int dy \int du \, \bar{n}_{ qi}(u) N_{i/A}(y) \delta(uy - \xi)
\]

\[
\xi^th_{\text{qi/A}} = \left\{ 1 + \frac{m_i^2 Q^2}{M^2 v^2} \right\}^{1/2} + 1 \bigg/ \left\{ 1 + \frac{Q^2}{v^2} \right\} + 1
\]

\[
\xi^th_{\text{qi/i}} = 2 \bigg/ \left\{ 1 + \frac{4m_i^2}{Q^2} \right\}^{1/2} + 1
\]

\[\bar{n}_{qi} \text{ from Regge behavior and counting rules (phase space)}\]

\[N_{i/A} \text{ from non-relativistic wave functions (NRWFs)}\]

\[p_i \text{ quark cluster probabilities evaluated from NRWFs}\]

based on critical separation of \(2 R_c \sim 1 \text{ fm}\)
DIS in the quark cluster model

Data: SLAC
Calculations: QCM

2%_FE / GAS_HE4 : E0 = 3.60  Theta = 25°
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.


See also: Proceedings of HUGS at CEBAF1992, & many conf. proceedings
DIS in the quark cluster model

Selected references:

H.J. Pirner and J.P. Vary,
"Deep-Inelastic Electron Scattering and the Quark Structure of $^3$He,"

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 $x > 1$]

M. Sato, S.A. Coon, H.J. Pirner and J.P. Vary,
"Quark Cluster Probabilities in Nuclei,"

A. Harindranath and J. P. Vary,
"Quark Cluster Model Predictions for the Nuclear Drell-Yan Process,"
Phys. Rev. D 34, 3378 (1986) [staircase function for $x > 1$ in DY]

G. Yen, J. P. Vary, A. Harindranath, and H. J. Pirner,
"Quark Cluster Model for Deep-Inelastic Lepton-Deuteron Scattering,"

H.J. Pirner and J.P. Vary,
“Boundary between hadron and quark/gluon structure of nuclei,"
Phys. Rev. C 84, 015201 (2011); nucl-th/1008.4962
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
Comparison between Quark-Cluster Model and JLAB data

and Phys. Rev. C 84, 015201 (2011); nucl-th/1008.4962;
Quark-cluster-model predictions for the nuclear Drell-Yan process

A. Harindranath and J. P. Vary

*Physics Department, Iowa State University, Ames, Iowa 50011*

(Received 8 April 1986)

We evaluate the quark-cluster-model predictions for lepton pair production in proton-nucleus, pion-nucleus, and nucleus-nucleus interactions. We examine the issue of a possible ambiguity between the $K$ factor and the probability of six-quark clusters in nuclei. We present predictions for cross sections and cross-section ratios which show substantial sensitivity to different features of the model. The model compares well with the existing data.

I. DY CROSS SECTION

In the hadron-hadron center-of-momentum frame we denote the total energy by $\sqrt{s}$. For hadrons $A$ and $B$ the four-momenta are $P_A=(\sqrt{s}/2,0,0,\sqrt{s}/2)$ and $P_B=(\sqrt{s}/2,0,0,-\sqrt{s}/2)$. Let $x_1$ ($x_2$) denote the fraction of longitudinal momentum carried by quark 1 (2) in hadron $A$ ($B$). Then the longitudinal momentum of the lepton pair with invariant mass $M$ is given by

$$P_L = p_1 + p_2 = (x_1 - x_2) \frac{\sqrt{s}}{2}.$$ 

$$\frac{d^2\sigma}{dx_1 dx_2} = \frac{4\pi\alpha^2}{9sx_1x_2} \sum e_q^2 F_q(x_1,x_2)$$

FIG. 7. QCM prediction for the ratio of DY cross sections for Fe and D as a function of $x_2$ (for $x_1=0.1$) in the region $0.1 \leq x_2 \leq 1.9$. 
Comparison of quark percolation with RHIC data


$\rho_h (fm^{-3})$  $\mu_\pi (GeV)$

- 0.17  0
- 0.46  0.12
- 0.46 (incl $\Delta'$s)  0.12

Nuclear saturation

Full percolation

Partial percolation
BLFQ study of QCD bound states -Yang Li, ISU PhD student

Hadrons are QCD bound states. In this study, we’ll focus on Λ baryon.

Setup the problem:

1. We adopt the previous symmetries and constraints;
2. Fock space truncation: |uds⟩ + |udsg⟩;
3. sector dependent renormalization, which has shown success in many-body computing [18].

Basic procedures:

1. Enumerate Fock space, within constraints and truncation;
2. Construct Hamiltonian matrix;
3. Diagonalize Hamiltonian, regularization and renormalization are essential for convergence;
4. Compute experimental observables
Vertices

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Renormalization is performed in $|uds\rangle$ sector.
some preliminary results

At continuum, physical observables should be independent to all regulators and HO natural length. We renormalize the ground state to physical mass of Λ(1116), and study the convergence of first excited state.

Colorlines: convergence of first excited state energy with different HO lengths $1/\sqrt{M_{\text{HO}} \Omega_{\text{HO}}}$. 

Colorlines: convergence of first excited state energy with odd/even $N_{\text{max}}$. ($1/\sqrt{M_{\text{HO}} \Omega_{\text{HO}}} = 1 \text{ fm}$)
some preliminary results

probability of finding a gluon in ground state:

~consistent with constituent quark model
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
- 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
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<td>Pieter Maris, Alina Negoita,</td>
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