I. Ab initio Hamiltonian approach to quantum many-body systems
II. Basis Light Front Quantization (BLFQ) - features of 2D HO
III. IR and UV regulators - a case study
IV. Zeroth order results and quantum statistical properties
V. Initial QED example with interactions in LF gauge
VI. Conclusions and Outlook
Collaborators on recent light-front projects

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Ab initio nuclear structure physics - fundamental questions

- What controls nuclear saturation?
- How does the nuclear shell model emerge from the underlying theory?
- What are the properties of nuclei with extreme neutron/proton ratios?
- Can nuclei provide precision tests of the fundamental laws of nature?
QCD
Theory of strong interactions

χEFT
Chiral Effective Field Theory

Inter-Nucleon
NN, NNN interactions
AV18, EFT, \textit{V}_{\text{low-k}}

Theory of Light Nuclei
Spectroscopy and selected reactions
Verification: NCSM+GMRCC
Validation: nuclei with \textit{A}>16

Density Functional Theory
Improved functionals
Remove computationally imposed constraints
Properties for all nuclei with \textit{A}>15

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

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

r,s processes
& Supernovae

Big Bang
Nucleosynthesis
& Stellar Reactions

UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

www.unedf.org
Fundamental Challenges

- What is the Hamiltonian
- How to renormalize to a finite basis space
- How to solve for non-perturbative observables
- How to take the continuum limit (IR -> 0, UV -> ∞)

Focii of the both the Nuclear Many-Body and Light-Front QCD communities!
Discretized Light Cone Quantization (c1985)

Basis Light Front Quantization

\[ \phi(\vec{x}) = \sum_{\alpha} \left[ f_\alpha(\vec{x}) a_\alpha^- + \frac{1}{f_\alpha}(\vec{x}) a_\alpha^- \right] \]

where \( \{a_\alpha\} \) satisfy usual (anti-) commutation rules.

Furthermore, \( f_\alpha(\vec{x}) \) are arbitrary except for conditions:

Orthonormal: \[ \int f_\alpha(\vec{x}) f_\alpha'(\vec{x}) d^3x = \delta_{\alpha\alpha'} \]

Complete: \[ \sum_{\alpha} f_\alpha(\vec{x}) f_\alpha'(\vec{x}') = \delta^3(\vec{x} - \vec{x}') \]

=> Wide range of choices for \( f_\alpha(\vec{x}) \) and our initial choice is

\[ f_\alpha(\vec{x}) = Ne^{ik^+x^-} \Psi_{n,m}(\rho,\varphi) = Ne^{ik^+x^-} f_{n,m}(\rho) \chi_m(\varphi) \]
ab initio Hamiltonian Methods

Problem Statement

Solve eigenvalue problem in large enough basis to converge

\[
H = H_0 + H_{\text{int}} \\
H \Psi_i = E_i \Psi_i \\
\Psi_i = \sum_{n=0}^{\infty} A_n^i \Phi_n \\
\text{Diagonalize} \{ \langle \Phi_m | H | \Phi_n \rangle \}
\]

Employ eigenvectors to calculate experimental observables

Transition Rate \((i \rightarrow k) \propto \left| \langle \Psi_i | \hat{O} | \Psi_k \rangle \right|^2 \)

Test fundamental strong interaction forces in nature
Test fundamental symmetries - standard model and beyond
What are the elements for solving the problem?

- Adopt a Hamiltonian & renormalize as needed - retain induced many-body interactions
- Adopt the 2-D Harmonic Oscillator (2DHO) + longitudinal DLCQ for basis states, \( \alpha, \beta, \ldots \)
- Evaluate the Hamiltonian, \( H \), in basis space of Fermion Slater determinants + Boson permanents (manages the bookkeeping of anti-symmetrization and symmetrization)

\[
|\Phi_n\rangle = [a_\alpha^+ \cdots a_\xi^+]_n |0\rangle
\]

- Diagonalize resulting sparse many-body \( H \) in this basis where

\( n = 1, 2, \ldots, 10^{10} \) or more!

- Evaluate observables and compare with experiment

\[
\text{Transition Rate } (i \rightarrow k) \propto |\langle \Psi_k | \hat{O} | \Psi_i \rangle|^2
\]

Comments:
- Straightforward but computationally demanding => new algorithms/computers
- Requires convergence assessments and extrapolation tools
- Achieved for nuclei up to \( A=16 \) (40) with largest computers available
- Basis is likely to be overcomplete but exact symmetries will be preserved
The properly normalized wavefunctions $\Psi_{n,m}(\rho, \phi) = f_{n,m}(\rho) \chi_m(\phi)$ are given by

$$f_{n,m}(\rho) = \sqrt{2 M \Omega} \frac{n!}{(n + |m|)!} e^{-M \Omega \rho^2/2} \left( \sqrt{M \Omega} \rho \right)^{|m|} L_n^{|m|}(M \Omega \rho^2)$$

$$\chi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

**Set of transverse 2D HO modes for n=0**

- $m=0$
- $m=1$
- $m=2$
- $m=3$
- $m=4$

J.P. Vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de Teramond, P. Sternberg, E.G. Ng and C. Yang, ArXiv:0905:1411
Set of transverse 2D HO modes for n=4

m=0

m=1

m=2

m=3

m=4

J.P. Vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de Teramond, P. Sternberg, E.G. Ng and C. Yang, ArXiv:0905:1411
\[ \Psi_{knm} = \psi_k(x^-)f_{nm}(\rho)\chi(\phi) \]

APBC: \[-L \leq x^- \leq L\]

\[ \psi_k(x^-) = \frac{1}{\sqrt{2L}} e^{i\pi \frac{x^-}{L}} \]

\[ k = \frac{1}{2}, \quad n = 1, \quad m = 0 \]
What motivates this BLFQ approach?

- Exact treatment of all symmetries (dynamical & kinematical)
- Success in ab-initio nuclear many-body theory (equal time, non-relativistic)
- High precision results from No-Core Full Configuration (NCFC) approach
- Advances in solving sparse matrix problems on parallel computers
- Growth in the size/capacity of parallel computers

Parameters of the HO basis space

Harmonic Oscillator with $\hbar\Omega^2/2 = 1$ "$\hbar\Omega$" configuration
Many Fermion Dynamics – nuclear physics

- MFDn: ab initio calculations for nuclear structure using basis space expansion methods
  - Variational: for any finite truncation of the basis space, MFDn gives an upper bound for the ground state energy
  - Smooth approach to asymptotic values with increasing basis space: no-core Full Configuration method

- Construct Many–Body Basis States in an \( m \)-scheme H.O. basis that eliminates spurious center of mass motion effects

- Construct the many-nucleon Hamiltonian in this basis
  - Determine which matrix elements are nonzero
  - Evaluate nonzero matrix elements

- Solve the many-nucleon Hamiltonian for lowest eigenvalues to obtain spectrum and wavefunctions (input for TRDENS)

- Evaluate selected 1-body and 2-body observables to compare with experiment and for use with energy-density functionals
Improvements to MFDn under SciDAC

Dimension

$13^c$ Chiral NN+NNN $- N_{max} = 6$ Basis Space

- **MFDn Version Date**
  - V10-B05 April 2007
  - V12-B00 October 2007
  - V12-B01 April 2008
  - V12-B09 January 2009

- **Input 3b matrix elements**
  - $3 \times 10^6$
  - $56 \times 10^{10}$
  - 3 Gbytes

- **Nonzero matrix elements**
  - $56 \times 10^{10}$
Demonstrate NCFC where one attains convergence directly or through extrapolation.
A-uses 4 successive $N_{\text{max}}$ points
B-uses 3 successive $N_{\text{max}}$ points

$\alpha + nn$ threshold

2.8 hours on 19,800 cores (Jaguar)

Vaintraub, Barnea & Gazit, arXiv0903.1048

| $\text{GT}_{\text{exp}}$ | 2.170 |
|------------------------|-------|
| $\text{GT}_{\text{thy}}$ | 2.225(2) |

P. Maris, J.P. Vary and A. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420
How accurately are resonant states predicted?

P. Maris, J.P. Vary and A. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420
P. Maris, J.P. Vary and A. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420
Established extrapolation for ground state and excited states

Results for $^6$Li with JISP16
- Spectrum in good agreement with experimental data
- Extrapolated spectrum nearly independent of basis space $\hbar \Omega$
  except for radially excited $J^\pi = 1^+$, $T = 0$ state
- Ground state quadrupole moment $Q$ also in good agreement

P. Maris, et al., to be published
Work in progress: A = 14 nuclei

14B, JISP16, Nmax = 0, 2, 4, 6 (hω = 10 to 40 MeV), 8 (hω = 17.5, 20.0, 22.5 MeV)

Extraction energy [MeV] (difference of extrapolated binding energies)

- * ground state J = 2
- J = 1
- J = 3
- J = 4

obtained on 30628 pe's on Jaguar at the NCCS
P. Maris, A. Shirokov, J. Vary

PRELIMINARY

- 9 hours on 30,628 cores (Jaguar) for 3 $\hbar\omega$ values
- w/o recent CS/AM improvements: 18 hrs / $\hbar\omega$ value
neutron droplets in external fields

\[ \frac{(E_{\text{tot}} - U_{\text{ext}})}{A} \text{ [MeV]} \]

- \( \hbar \Omega = 40 \text{ MeV} \)
  - 8 neutrons, JISP16
  - 8 n, N3LO_{SRG}[\lambda=1.5]

- \( \hbar \Omega = 20 \text{ MeV} \)
  - 20 neutrons, JISP16
  - 20 n, N3LO_{SRG}[\lambda=1.5]

- \( \hbar \Omega = 5 \text{ MeV} \)

radius [fm]

P. Maris, et al., to be published
ab initio NCFC: UV and IR regulators in 3D HO basis space

\[ \Lambda = \sqrt{m_N \Omega (N + 3/2)} \quad \text{and} \quad \lambda = \sqrt{m_N \Omega / (N + 3/2)} \]

where

\[ N = \text{Max}\{2n + l\} \] in many - body basis states,

\[ N_0 = 2n + l \] of highest sp orbit in the lowest many - body basis state, and

\[ N_{\text{max}} = N - N_0. \]

Ideally, \( \Lambda \geq \Lambda \nu \), where \( \Lambda \nu = \) UV regulator of the interactions

Typically, \( \Lambda \nu \approx 600\text{MeV/c} \)

Ideally also, we strive to achieve independence of \( \lambda \), as \( \lambda \to 0 \)

S. Coon, et al., to be published

BLFQ: UV and IR regulators in transverse 2D HO basis space

\[ \Lambda = \sqrt{M_0 \Omega (N + 1)} \quad \text{and} \quad \lambda = \sqrt{M_0 \Omega / (N + 1)} \]

where

\[ N = \text{Max}\{2n + |m|\} \] in many - parton basis states,

\[ N_0 = 2n + |m| \] of highest sp orbit in the lowest many - parton basis state, and

\[ N_{\text{max}} = N - N_0 = N \] (forseeable future)

Ideally, \( \Lambda \geq \Lambda \nu \), where \( \Lambda \nu = \) UV regulator of the interactions

Ideally also, we strive to achieve independence of \( \lambda \), as \( \lambda \to 0 \)
$^2\text{H}$

Oscillator Energy (MeV)
- 10
- 20
- 30
- 40
- 50

Ground State Energy (MeV)

$N_{\text{max}} = 6 - 60$ fitted

$2.224575 + a \exp(-c\lambda^2) + b\lambda^d$

S. Coon, et al., to be published
BLFQ Symmetries and Constraints

Explicit but flexible symmetries/constraints
Flexible => all but first are input selections
Items in red are new/revised in last 12 months

• Identical particle statistics of Fermions and Bosons
• Total baryon number = B
• Total charge = Z
• Total SU(3) color singlet basis space constructed
• Total angular momentum projection $J_z = M + S$
• Total number of q-qbar pairs or limited only by $(N_{\text{max}}, K)$
• Total number of gluons or limited only by $(N_{\text{max}}, K)$

Symmetries/constraints via Lagrange method
Total transverse momentum eliminated by exact factorization of the light-front wavefunction
Symmetries & Constraints

\[ \sum_i b_i = B \]
\[ \sum_i (m_i + s_i) = J_z \]
\[ \sum_i k_i = K \]
\[ \sum_i [2n_i + |m_i| + 1] \leq N_{\text{max}} \]

Global Color Singlets (QCD)
Light Front Gauge
Optional - Fock space cutoffs

Finite basis regulators
Hamiltonian for “cavity mode” QCD in the chiral limit

Why interesting - cavity modes of AdS/QCD

\[ H = H_0 + H_{\text{int}} \]

Massless partons in a 2D harmonic trap solved in basis functions commensurate with the trap:

\[ H_0 \equiv 2M_0 P_c^\pm = \frac{2M_0 \Omega}{K} \sum_i \frac{1}{x_i} [2n_i + |m_i| + 1] \]

with \( \Lambda \lambda \) defining the confining scale as well as the basis function scale.

Initially, we study this toy model of harmonically trapped partons in the chiral limit on the light front. Note \( Kx_i = k_i \) and BC's will be specified.
Quantum statistical mechanics of trapped systems in BLFQ: Microcanonical Ensemble (MCE)

Develop along the following path:

Select the trap shape (transverse 2D HO)
Select the basis functions (BLFQ)
Enumerate the many-parton basis in unperturbed energy order dictated by the trap - obeying all symmetries
Count the number of states in each energy interval that corresponds to the experimental resolution $\Rightarrow$ state density
Evaluate Entropy, Temperature, Pressure, Heat Capacity, Gibbs Free Energy, Helmholtz Free Energy, . . .

Note: With interactions, we will remove the trap and examine mass spectra and other observables.
Microcanonical Ensemble (MCE) for Trapped Partons

Solve the finite many-body problem:

\[ H|\Psi_i\rangle = E_i |\Psi_i\rangle \]

and form the density matrix:

\[ \rho(E) \equiv \sum_{i \in E_i = E \pm \Delta} |\psi_i\rangle \langle \psi_i| \]

Statistical Mechanical Observables:

\[ \langle O \rangle = \frac{\text{Tr}(\rho O)}{\text{Tr}(\rho)} \]

\[ \text{Tr}(\rho) \equiv \Gamma(E) = \text{Total number of states in MCE at } E \]

\[ \Gamma(E) \equiv \omega(E)\Delta \]

\[ \omega(E) \equiv \text{Density of states at } E \]

\[ S(E,V) \equiv k \ln(\Gamma(E)) \]

\[ \frac{1}{T} \equiv \frac{\partial S}{\partial E}; \quad P \equiv T \left( \frac{\partial S}{\partial V} \right)_E; \quad C_V \equiv \left( \frac{\partial E}{\partial T} \right) \]
Basis Light Front Quantized (BLFQ) Field Theory

- Choose a set of parton basis states in LF coordinates
- Enumerate many-parton basis states up to chosen cutoff
- Select the LF gauge
- Evaluate $H_{QFT}$ in that basis - regulate/renormalize
- Diagonalize to obtain mass spectrum and LF amplitudes
- Evaluate experimental observables

$B = 0$ cavity mode states

J.P. Vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de Teramond, P. Sternberg, E.G. Ng and C. Yang, ArXiv:0905:1411
J.P. Vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de Teramond, P. Sternberg, E.G. Ng and C. Yang, ArXiv:0905:1411
J.P. Vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de Teramond, P. Sternberg, E.G. Ng and C. Yang, ArXiv:0905:1411
Cavity mode QED with no net charge & $K = N_{\text{max}}$
Distribution of multi-parton states by Fock-space sector

| $\bar{f} f$ pairs / bosons | 0   | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  | Total |
|-----------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|
| 0                           | 0   | 0   | 210 | 0   | 1122| 0   | 67  | 0   | 1   | 0   | 0   | 1400  |
|                             | 0   | 0   | 495 | 0   | 11318| 0   | 2936| 0   | 69  | 0   | 1   | 14819 |
|                             | 0   | 0   | 1001| 0   | 73600| 0   | 63315| 0   | 4027| 0   | 69  | 142013|
| 1                           | 420 | 1932| 8190| 1040| 588 | 8   | 2   | 0   | 0   | 0   | 0   | 12180 |
|                             | 990 | 10512| 86856| 33632| 36672| 1604| 640 | 8   | 2   | 0   | 0   | 170916|
|                             | 2362| 40810| 574800| 503940| 929064| 99962| 60518| 1770| 644 | 8   | 2   | 2212680|
| 2                           | 5961| 1500| 1339| 4   | 1   | 0   | 0   | 0   | 0   | 0   | 0   | 8559  |
|                             | 64240| 59240| 97584| 4040| 1513| 4   | 1   | 0   | 0   | 0   | 0   | 226622|
|                             | 127730| 942240| 2806624| 381608| 249825| 4928| 1565| 4   | 1   | 0   | 0   | 4814525|
| 3                           | 218 | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 218   |
|                             | 25584| 1528| 554 | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 27666  |
|                             | 808034| 222336| 200676| 2592| 602 | 0   | 0   | 0   | 0   | 0   | 0   | 1234240|
| 4                           | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0     |
|                             | 16  | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 16    |
|                             | 18325| 168 | 20  | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 19513  |

J.P. Vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de Teramond, P. Sternberg, E.G. Ng and C. Yang, ArXiv:0905:1411
Non-interacting QED cavity mode with zero net charge
Photon distribution functions

Labels: $N_{\text{max}} = K_{\text{max}} \sim Q$

“Weak” coupling:
Equal weight to low-lying states

“Strong” coupling:
Equal weight to all states

J.P. Vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de Teramond, P. Sternberg, E.G. Ng and C. Yang, ArXiv:0905:1411
Elementary vertices in LF gauge

QED & QCD

\[ H_{\text{QED}} \]

QCD
Renormalization in BLFQ => Analyze divergences

➢ Are matrix elements finite - No => counterterms
➢ Are eigenstates convergent as regulators removed?

Examine behavior of off-diagonal matrix elements of the vertex for the spin-flip case:
As a function of the 2D HO principal quantum number, n.
Second order perturbation theory gives log divergence if such a matrix element goes as $1/\sqrt{n+1}$

J.P. Vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de Teramond, P. Sternberg, E.G. Ng and C. Yang, ArXiv:0905:1411
Cavity mode QED

\[ M_0 = \Omega = m_e = 1 \]
\[ K = 3, \quad N_{\text{max}} = 2, \quad M_j = 1/2 \]
\[ g_{\text{QED}} = [4\pi \alpha]^{1/2} \]

lepton & lepton-photon Fock space only

Next steps

- Increase basis space size
- Evaluate anomalous magnetic moment
- Remove cavity

H. Honkanen, et al., to be published
Conclusions and Outlook

- Progress in line with Ken Wilson’s advice = adopt MBT advances
- Exact treatment of all symmetries is challenging but doable
- Important progress in managing IR and UV cutoff dependences
- Advances in algorithms and computer technology crucial
- First results with interaction terms in QED - anomalous moment
- Community effort welcome to advance the field dramatically