Ab initio Nuclear Physics from Hadrons to Nuclei

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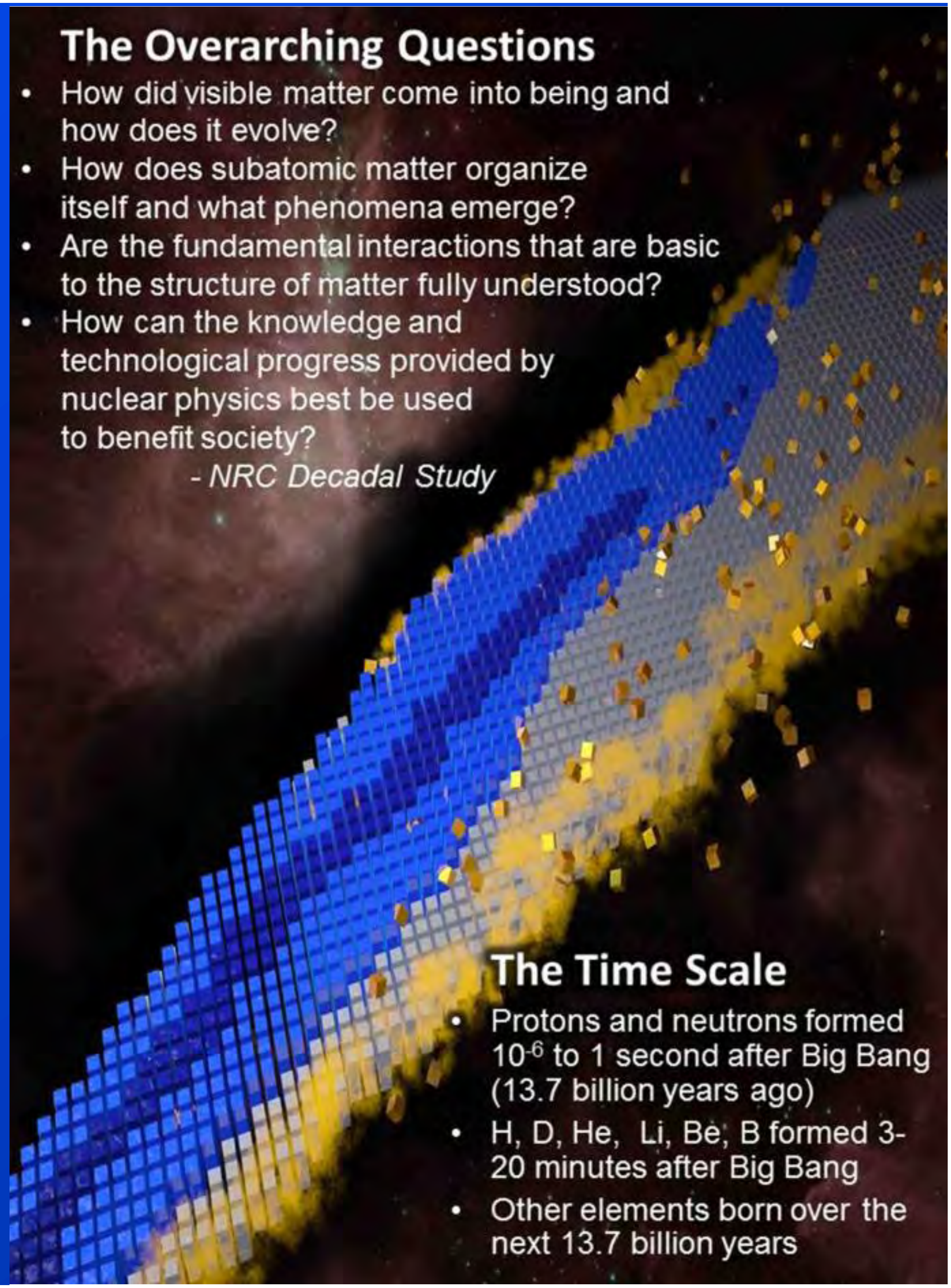
Nuclear Theory
in the
Supercomputer Era
(NTSE-2024)

Busan
South Korea

December 6, 2024



Standard Model is the current starting point
for describing the nuclear processes
that brought the universe to the present time
and can provide fusion energy for the future

This starting point defines our "ab initio"
or "from the beginning" theory of the atomic nucleus

Can we successfully proceed from that starting point
to explain/predict nuclear phenomena and use
discrepancies with experiment to reveal new physics?

Starting point: QCD Lagrangian

Lattice Gauge theory

Feynman Covariant Perturbation Theory

Hamiltonian Field Theory

Covariant Wave Equations

Steps to set up non-perturbative calculational framework	*Specific selections for these applications*
Make Legendre Transform	L --> $T^{\mu\nu}$ Energy-Momentum tensor
Select a coordinate system	Light-Front coordinates & identify generators
Fix the Gauge	Light-Front Gauge ($A^+ = 0$)
Eliminate dependent fields	Dirac -> Pauli fields
Select basis for the fields	2D HO + Jacobi Polynomials or DLCQ
Quantize the theory	Basis Light-Front Quantization (BLFQ)
Select cutoffs	N_{max}, L or K, Fock space limits
Evaluate/store Hamiltonian matrix	High-Performance Computers (HPCs)
Solve for eigenpairs (mass states & Light-Front Wavefunctions (LFWFs))	High-Performance Computers (HPCs)
Solve for experimental observables	Matrix elements of operators with LFWFs

Dirac's forms of relativistic dynamics [Dirac, Rev. Mod. Phys. **21**, 392 1949]

Instant form is the well-known form of dynamics starting with $x^0 = t = 0$

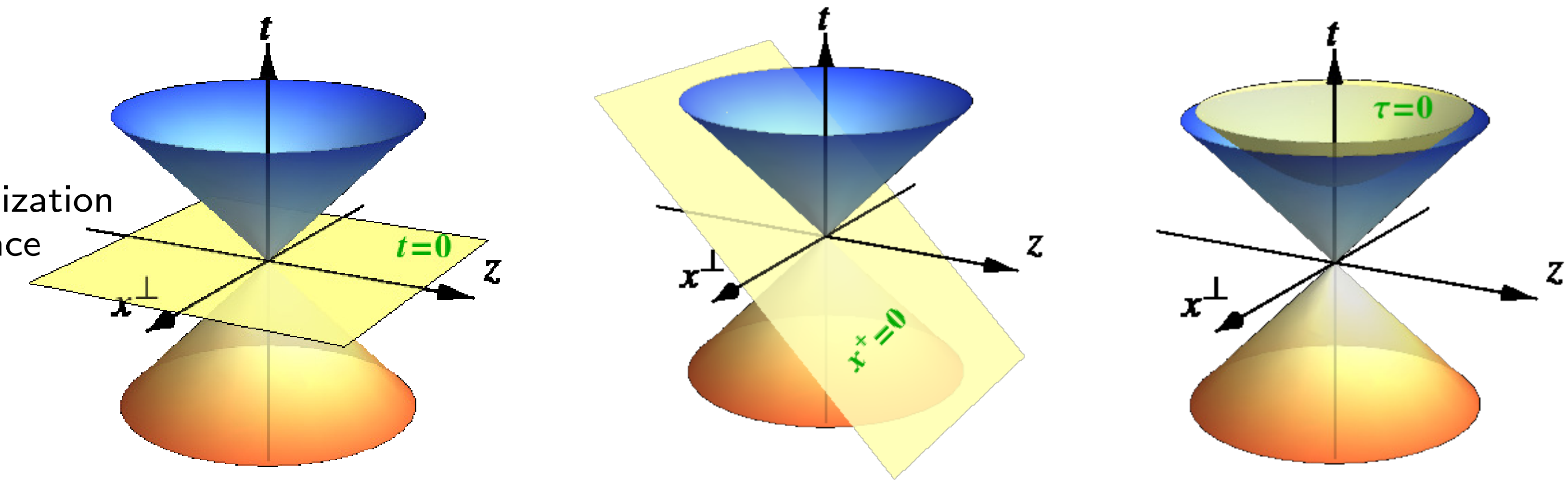
$K^i = M^{0i}$, $J^i = \frac{1}{2}\varepsilon^{ijk}M^{jk}$, ε^{ijk} = (+1,-1,0) for (cyclic, anti-cyclic, repeated) indeces

Front form defines relativistic dynamics on the light front (LF): $x^+ = x^0 + x^3 = t + z = 0$

$$P^{\pm} \triangleq P^0 \pm P^3,\ \vec{P}^{\perp} \triangleq (P^1, P^2),\ x^{\pm} \triangleq x^0 \pm x^3,\ \vec{x}^{\perp} \triangleq (x^1, x^2),\ E^i = M^{+i},$$
$$E^+ = M^{+-},\ F^i = M^{-i}$$

	instant form	front form	point form
time variable	$t = x^0$	$x^+ \triangleq x^0 + x^3$	$\tau \triangleq \sqrt{t^2 - \vec{x}^2 - a^2}$

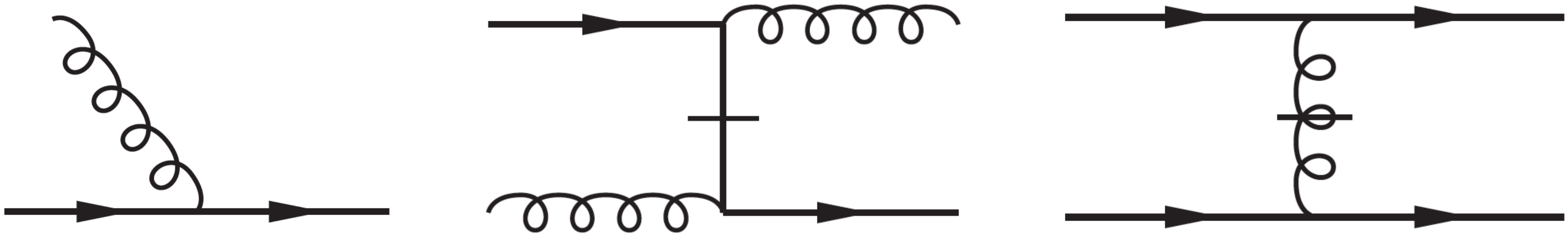
quantization surface



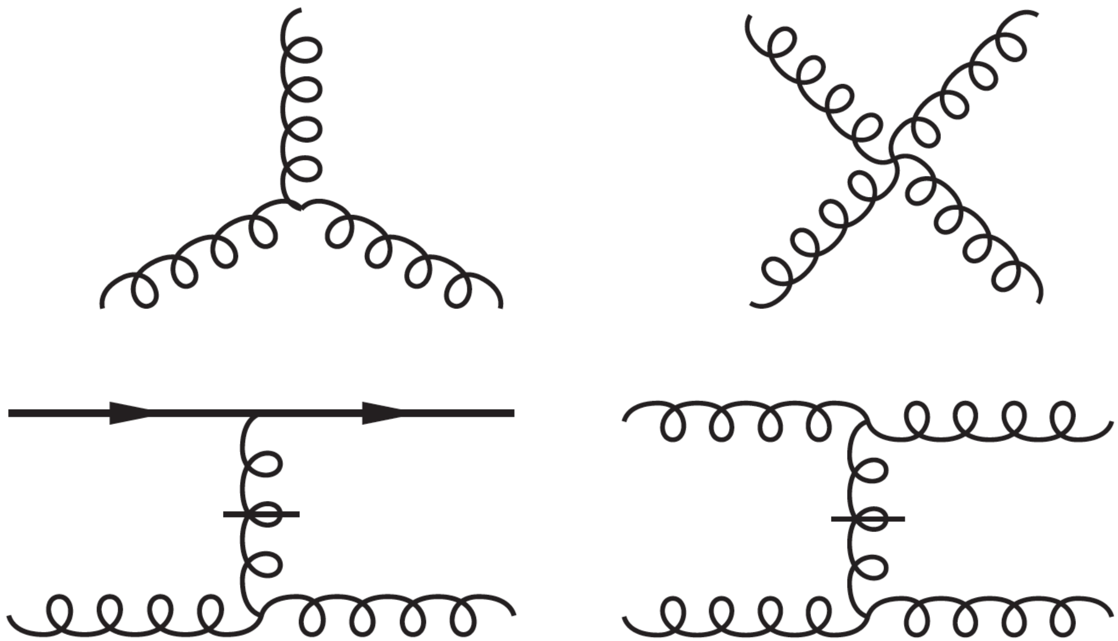
	instant form	front form	point form
Hamiltonian	$H = P^0$	$P^- \triangleq P^0 - P^3$	P^μ
kinematical	$\vec{P}, \vec{J}$	$\vec{P}^{\perp}, P^+, \vec{E}^{\perp}, E^+, J^-$	$\vec{J}, \vec{K}$
dynamical	$\vec{K}, P^0$	$\vec{F}^{\perp}, P^-$	$\vec{P}, P^0$
dispersion relation	$p^0 = \sqrt{\vec{p}^2 + m^2}$	$p^- = (\vec{p}_{\perp}^2 + m^2)/p^+$	$p^\mu = mv^\mu\ (v^2 = 1)$

Adapted from talk by Yang Li

Light Front (LF) Hamiltonian Defined by its Elementary Vertices in LF Gauge



QED & QCD



QCD

Discretized Light Cone Quantization

[H.C. Pauli & S.J. Brodsky, PRD32 (1985)]

Basis Light Front Quantization

[J.P. Vary, …**P. Maris**, … **E.G. Ng**, et al., PRC81 (2010)]

$$\phi\left(\vec{k}_\perp, x\right) = \sum_\alpha \left[f_\alpha\left(\vec{k}_\perp, x\right) a_\alpha + f_\alpha^*\left(\vec{k}_\perp, x\right) a_\alpha^\dagger \right]$$

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

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

Orthonormal: $$\int f_\alpha\left(\vec{k}_\perp, x\right) f_{\alpha'}^*\left(\vec{k}_\perp, x\right) \frac{d^2 k_\perp dx}{(2\pi)^3 2x(1-x)} = \delta_{\alpha\alpha'}$$

Complete: $$\sum_\alpha f_\alpha\left(\vec{k}_\perp, x\right) f_\alpha^*\left(\vec{k}'_\perp, x'\right) = 16\pi^3 \sqrt{x(1-x)}\,\delta^2\left(\vec{k}_\perp - \vec{k}'_\perp\right)\delta\left(x - x'\right)$$

For mesons we adopt (later extended to baryons): [Y. Li, et al., PLB758 (2016)]

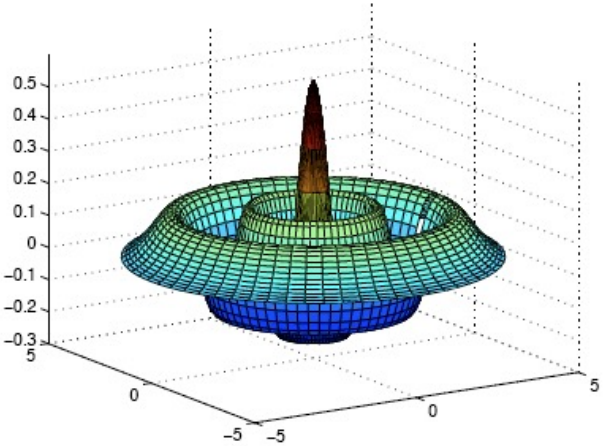
$$f_{\alpha=\{nml\}}\left(\vec{k}_\perp, x\right) = \phi_{nm}\left(\vec{k}_\perp / \sqrt{x(1-x)}\right)\chi_l\left(x\right)$$

ϕ_{nm} 2D-HO functions as in AdS/QCD

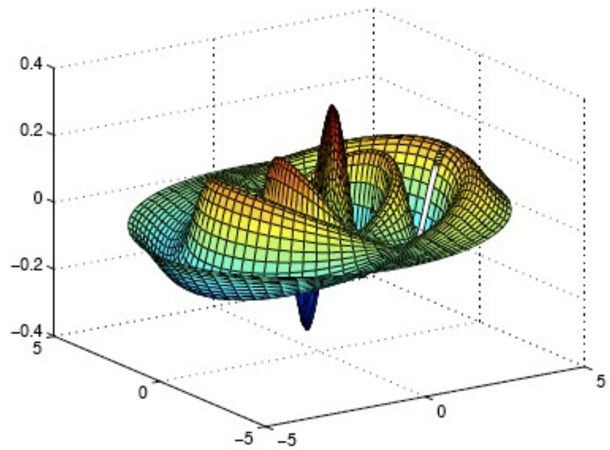
χ_l Jacobi polynomials times $x^a(1-x)^b$

Set of Transverse 2D HO Modes for n=4

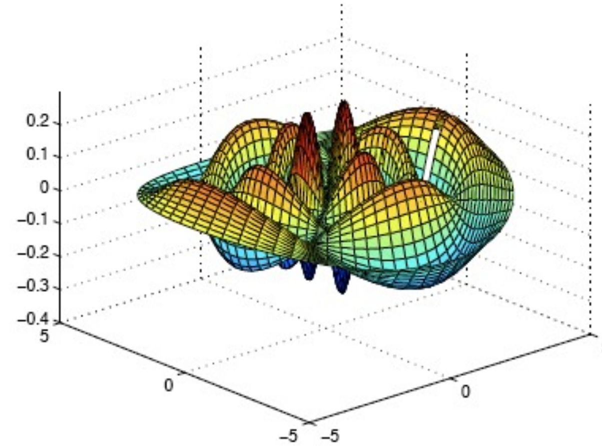
m=0



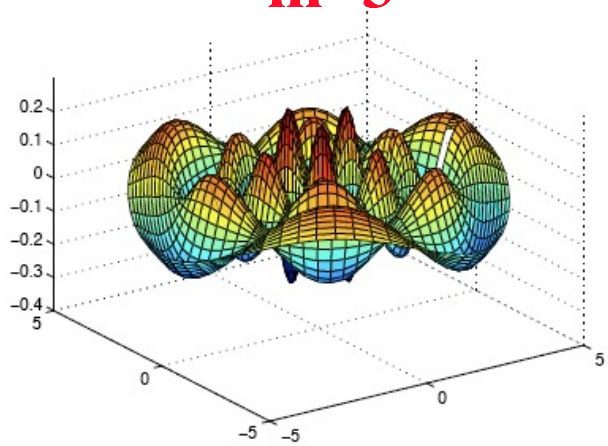
m=1



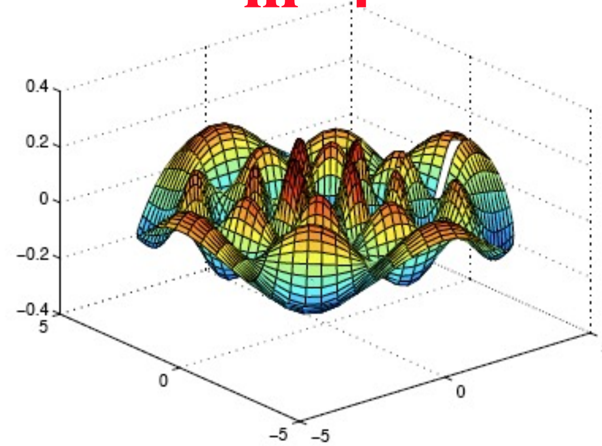
m=2



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, PRC 81, 035205 (2010)

BLFQ
Symmetries & Constraints

All $J \geq J_z$ states in one calculation

Finite basis regulators

Preserve transverse boost invariance

Baryon number $\sum_i b_i = B$

Charge $\sum_i q_i = Q$

Angular momentum projection (M-scheme) $\sum_i (m_i + s_i) = J_z$

Longitudinal momentum (Bjorken sum rule) $\sum_i x_i = \sum_i \frac{k_i}{K} = 1$

Longitudinal mode regulator (Jacobi) $\sum_i l_i \leq L$

Transverse mode regulator (2D HO) $\sum_i (2n_i + |m_i| + 1) \leq N_{\max}$

"Internal coordinates" $\vec{k}_{i\perp} = \vec{p}_{i\perp} - x_i \vec{P}_\perp \quad \Rightarrow \quad \sum_i \vec{k}_{i\perp} = 0$

$H \to H + \lambda H_{CM}$

Global Color Singlets (QCD)

Light Front Gauge

Optional Fock-Space Truncation

Light-Front Wavefunctions (LFWFs)

$$|\psi_h(P,j,\lambda)\rangle = \sum_n \int [\mathrm{d}\mu_n]\, \psi_{n/h}(\{\vec{k}_{i\perp}, x_i, \lambda_i\}_n) |\{\vec{p}_{i\perp}, p_i^+, \lambda_i\}_n\rangle$$

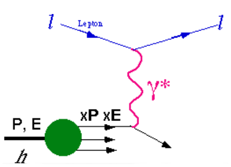
LFWFs are *frame-independent* (boost invariant) and depend only on the relative variables: $x_i \equiv p_i^+/P^+, \vec{k}_{i\perp} \equiv \vec{p}_{i\perp} - x_i \vec{P}_\perp$

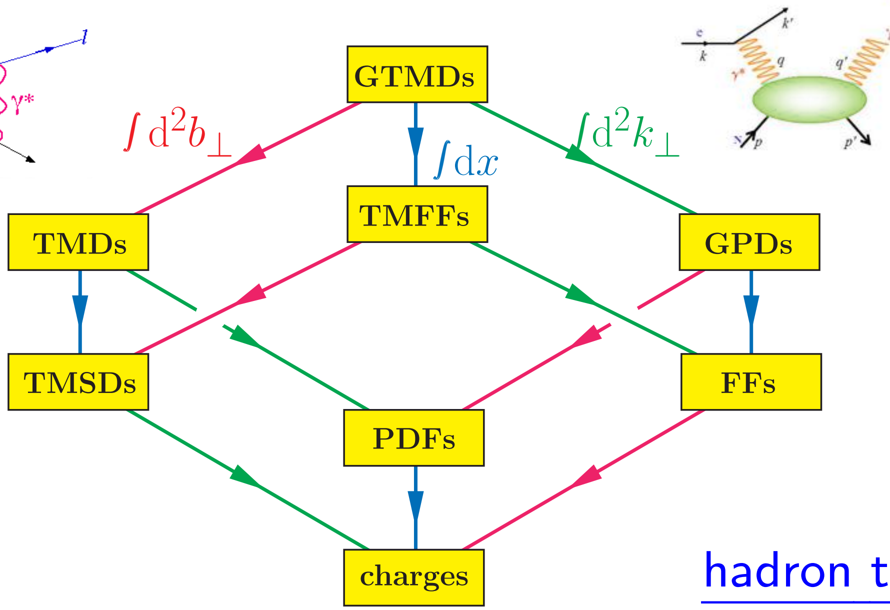
LFWFs provide intrinsic information of the structure of hadrons, and are indispensable for exclusive processes in DIS [Lepage '80]

- Overlap of LFWFs: structure functions (e.g. PDFs), form factors, ...
- Integrating out LFWFs: light-cone distributions (e.g. DAs)

"Hadron Physics without LFWFs is like Biology without DNA!"

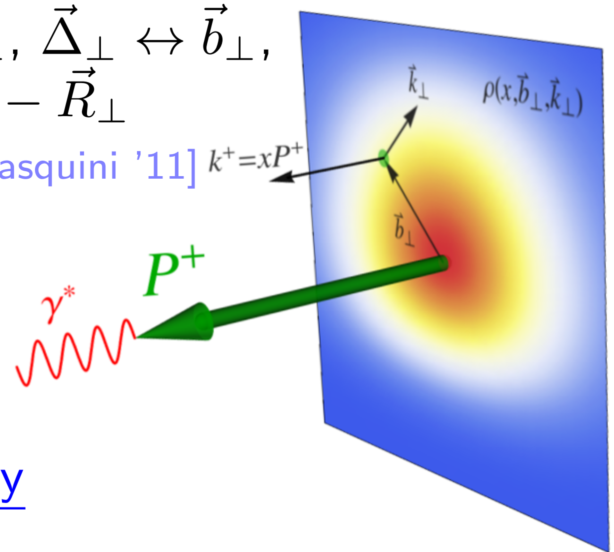
— Stanley J. Brodsky





$\vec{k}_\perp \leftrightarrow \vec{r}_\perp$, $\vec{\Delta}_\perp \leftrightarrow \vec{b}_\perp$,
$\vec{b}_\perp = \vec{r}_\perp - \vec{R}_\perp$

[Lorcé & Pasquini '11]



hadron tomography

Research results from BLFQ as of LC2024

- There have been ~60 papers on BLFQ and tBLFQ from 2010 – present.
  Of these, 48 have either “Basis Light-Front Quantization” or “BLFQ” in the title.

- Since 2020, the “BLFQ Collaboration” has posted ~ 30 papers on the arXiv
  and has ~27 published plus accepted papers.

- This year, to date, the BLFQ Collaboration has posted 9 papers to the arXiv:
  6 have been published and 3 are submitted for publication.

- LC-2024 Talks – Yiping Liu, Tianyang Hu, Chandan Mondal, Meijian Li,
  Wenyang Qian, Sreeraj Nair, Zhi Hu, Satvir Kaur, Lingdi Meng, Tiancai Peng, . . .

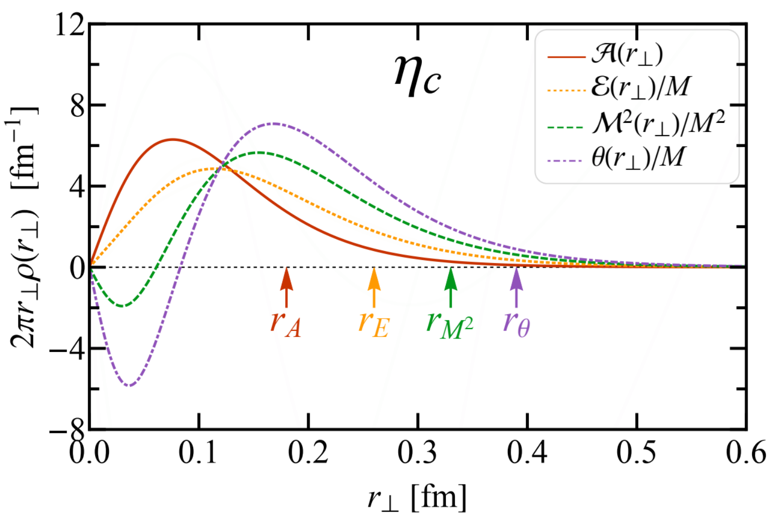
- NTSE-2024 Talks – Mondal, Zhao, Vary

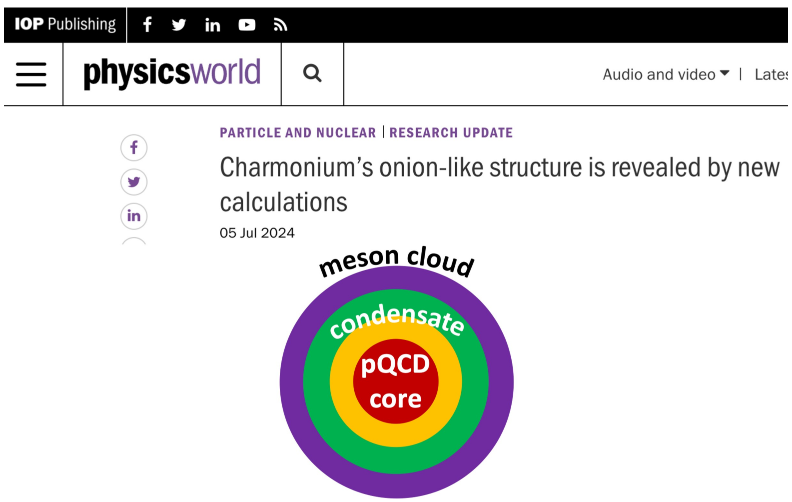
Physical densities

- Different physical densities: matter density $\mathcal{A}(r_\perp)$, energy density $\mathcal{E}(r_\perp)$, invariant mass squared density $\mathcal{M}^2(r_\perp)$ and scalar density $\theta(r_\perp) = \mathcal{T}^\alpha_{\ \alpha}(r_\perp) = \mathcal{E}(r_\perp) - 3\mathcal{P}(r_\perp)$
- Because of $D < 0$, there is a chain of inequalities about their root mean square radii

$$r_A < r_E < r_{M^2} < r_\theta$$

where,
$r_A^2 = -6A'(0)$, $r_E^2 = r_A^2 - \frac{3}{2}\lambda_C^2(1+D)$, $r_{M^2}^2 = r_A^2 - \frac{3}{2}\lambda_C^2(1+2D)$, $r_\theta^2 = r_A^2 - \frac{3}{2}\lambda_C^2(1+3D)$





Tianyang Hu, Xianghui Cao, Siqi Xu, Yang Li, Xingbo Zhao and James P. Vary, arXiv: 2408.09689

BLFQ Basis States

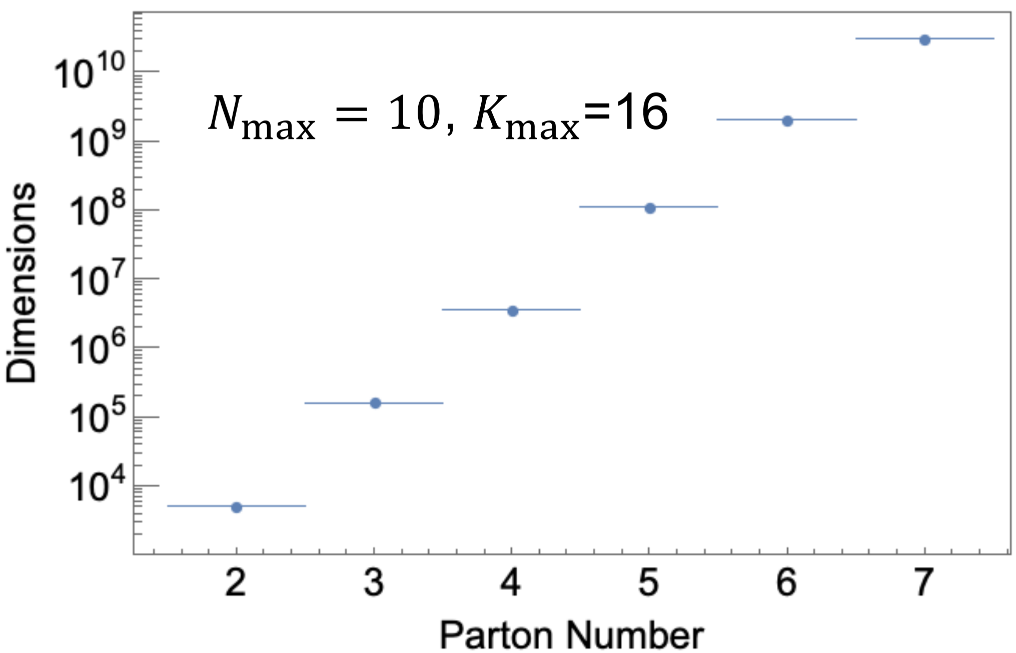
- BLFQ basis: expansion in Fock space beyond the valence sector

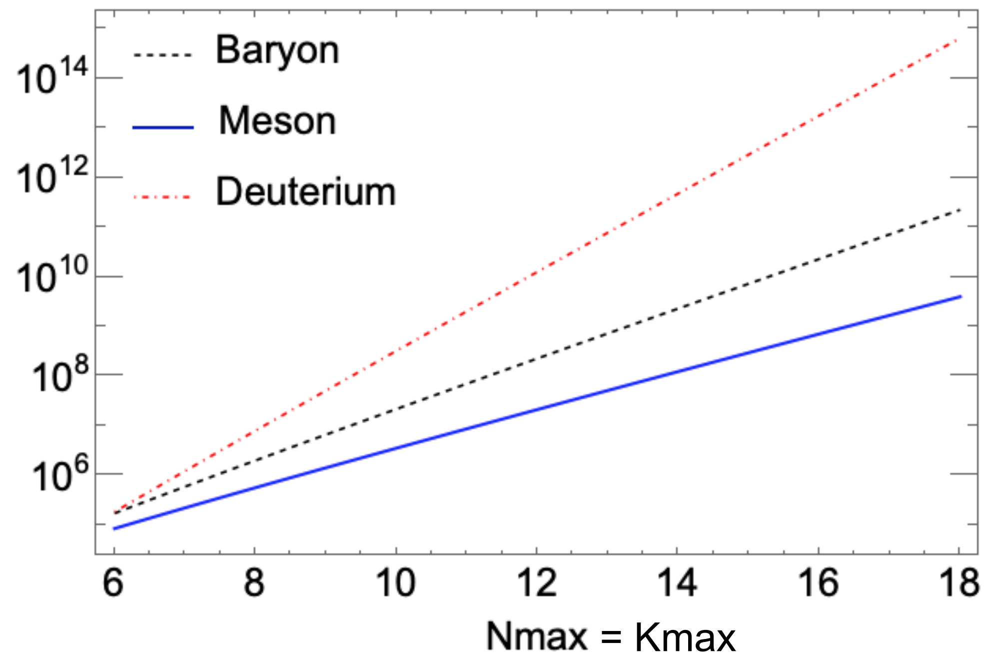
$$|\beta_{\text{meson}}\rangle = |q\bar{q}\rangle + |q\bar{q}g\rangle + |gg\rangle + |q\bar{q}\ q\bar{q}\rangle + |q\bar{q}\ gg\rangle + |q\bar{q}\ q\bar{q}\ g\rangle + |q\bar{q}q\bar{q}gg\rangle + \cdots$$

$$|\beta_{\text{baryon}}\rangle = |qqq\rangle + |qqqg\rangle + |qqq\ q\bar{q}\rangle + |qqq\ gg\rangle + |qqq\ q\bar{q}g\rangle + |qqqq\bar{q}gg\rangle + \cdots$$

$$|\beta_{\text{deuterium}}\rangle = |qqq\ qqq\rangle + |qqq\ qqq\ g\rangle + |qqq\ qqq\ q\bar{q}\rangle + |qqq\ qqq\ gg\rangle + \cdots$$

- Dimension of basis states increases with number of Fock sectors
  => motivation for quantum computing





Dimension of Basis States

- Expansion in BLFQ basis

$$|N\rangle = |qqq\rangle + |qqqg\rangle + |qqq\, q\bar{q}\rangle + |qqq\, gg\rangle + |qqq\, ggg\rangle + |qqq\, q\bar{q}\, g\rangle$$

$N_{max} = 7, K_{max} = 16$

	$\|qqq\rangle$	$\|qqqg\rangle$	$\|qqq\, q\bar{q}\rangle$	$\|qqq\, gg\rangle$	$\|qqq\, ggg\rangle$	$\|qqq\, q\bar{q}\, g\rangle$
dimension	35,088	592,960	3,901,500	5,169,360	19,603,584	7,128,576
Color	1	2	3	6	22	8

$$|N\rangle = |qqq\rangle + |qqqg\rangle + |qqq\, u\bar{u}\rangle + |qqq\, d\bar{d}\rangle + |qqq\, s\bar{s}\rangle$$

Basis Dimension= 12,332,548

$$|N\rangle = |qqq\rangle + |qqqg\rangle + |qqq\, u\bar{u}\rangle + |qqq\, d\bar{d}\rangle + |qqq\, s\bar{s}\rangle + |qqq\, gg\rangle$$

Basis Dimension= 17,501,908

$$|N\rangle = |qqq\rangle + |qqqg\rangle + |qqq\, q\bar{q}\rangle + |qqq\, gg\rangle + |qqq\, ggg\rangle$$

Basis Dimension= 37,105,492

$$|N\rangle = |qqq\rangle + |qqqg\rangle + |qqq\, q\bar{q}\rangle + |qqq\, gg\rangle + |qqq\, ggg\rangle + |qqq\, q\bar{q}\, g\rangle$$

Basis Dimension= 58,491,220

Full BLFQ

$$|N\rangle \rightarrow |qqq\rangle + |qqqg\rangle + |qqqu\bar{u}\rangle + |qqqd\bar{d}\rangle + |qqqs\bar{s}\rangle + |qqqgg\rangle$$

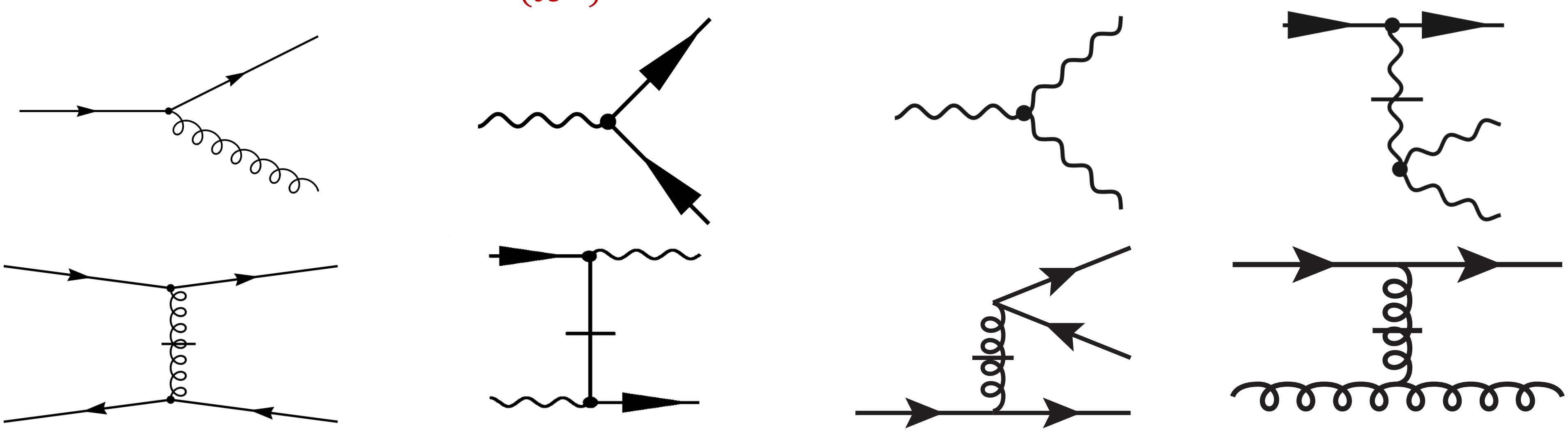
$$P^- = H_{K.E.} + H_{Interact}$$

Preliminary
Further progress towards first principles

$$H_{K.E.} = \sum_i \frac{p_i^2 + m_q^2}{p_i^+}$$

$$H_{Interact} = g\bar{\psi}\,\gamma^\mu T^a\,\psi\,A_\mu^a + \frac{g^2 C_F}{2}\,j^+ \frac{1}{(i\partial^+)^2} j^+ + \frac{g^2 C_F}{2}\,\bar{\psi}\gamma^\mu A_\mu \frac{\gamma^+}{i\partial^+} A_\nu \gamma^\nu \psi$$

$$-g^2 C_F \bar{\psi}\gamma^+\psi \frac{1}{(i\partial^+)^2}\, i\partial^+ A_\mu^a A_b^\mu + igf^{abc} i\partial^\mu A_a^\nu A_\mu^b A_\nu^c$$



Fock Sector Decomposition

$$|P_{baryon}\rangle \rightarrow |qqq\rangle + |qqqg\rangle + |qqqu\bar{u}\rangle + |qqqd\bar{d}\rangle + |qqqs\bar{s}\rangle + |qqqgg\rangle$$

$|qqq\,q\bar{q}\rangle \sim$ 3 color singlet state

1 singlet ⊗ singlet

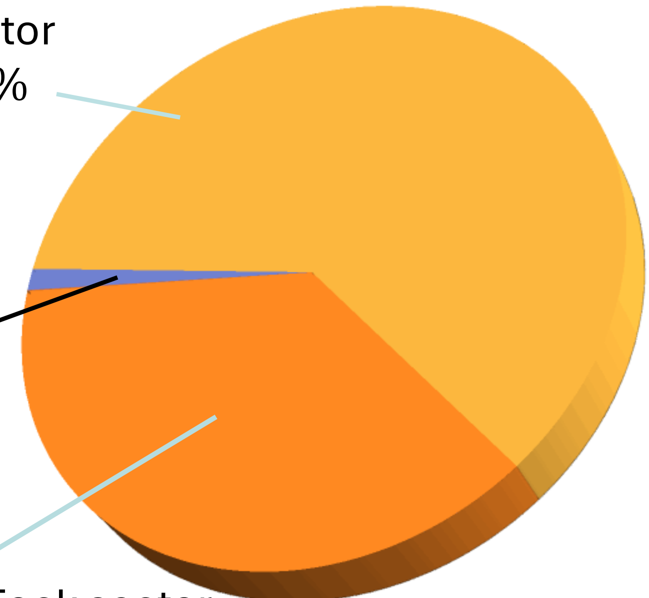
2 octet ⊗ octet

$|qqq\,gg\rangle \sim$ 6 color singlet state

1 singlet ⊗ singlet

4 octet ⊗ octet

1 decuplet ⊗ octet ⊗ octet



m_u	m_d	m_s	m_f	g	b	b_{inst}
0.5 GeV	0.45 GeV	0.6 GeV	3.0 GeV	2.1	0.6 GeV	3.0 GeV

Truncation parameter: $N_{\max} = 7$ and $K_{\max} = 10$

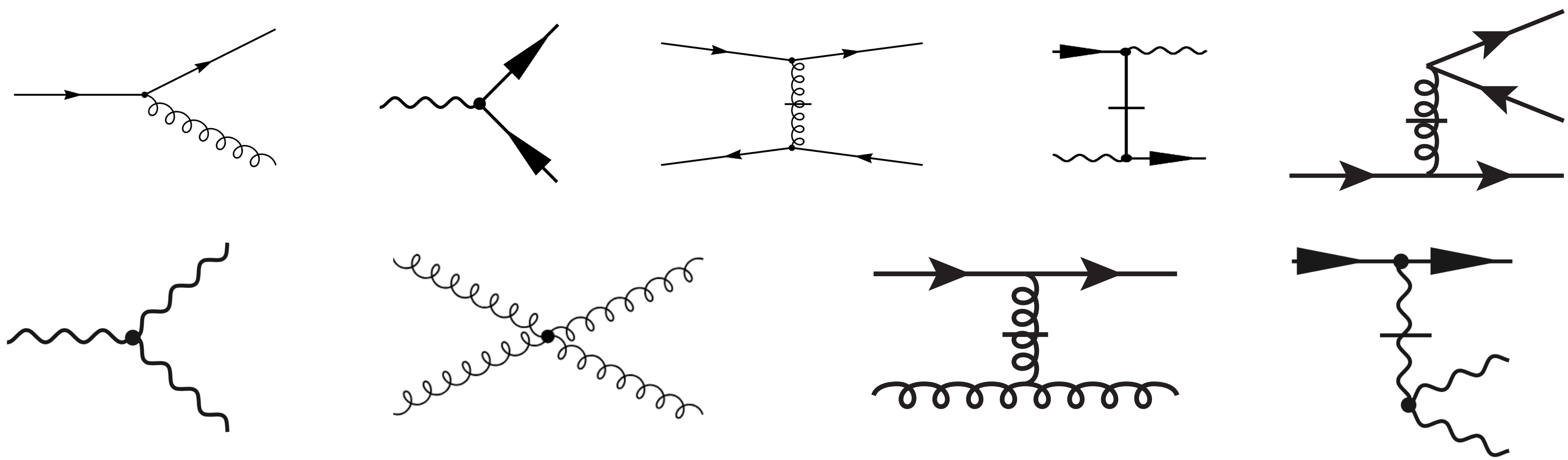
Next step in approach to Full BLFQ

$$|N\rangle \rightarrow |qqq\rangle + |qqqu\bar{u}\rangle + |qqqd\bar{d}\rangle + |qqqs\bar{s}\rangle + |qqqg\rangle + |qqqgg\rangle + |qqqggg\rangle$$

$$P^- = H_{K.E.} + H_{Interact} \qquad H_{K.E.} = \sum_i \frac{p_i^2 + m_q^2}{p_i^+}$$

$$H_{Interact} = g\bar{\psi}\,\gamma^\mu T^a\,\psi\,A_\mu^a + \frac{g^2 C_F}{2}\,j^+ \frac{1}{(i\partial^+)^2} j^+ + \frac{g^2 C_F}{2}\,\bar{\psi}\gamma^\mu A_\mu \frac{\gamma^+}{i\partial^+} A_\nu \gamma^\nu \psi$$

$$-g^2 C_F \bar{\psi}\gamma^+\psi \frac{1}{(i\partial^+)^2} i\partial^+ A_\mu^a A_b^\mu + igf^{abc} i\partial^\mu A_a^\nu A_\mu^b A_\nu^c + \frac{1}{4} g^2 f^{abc} f^{ade} A_b^\mu A_c^\nu A_{\mu d} A_{\nu e}$$



Fock Sector Decomposition

$$|P_{baryon}\rangle \rightarrow |qqq\rangle + |qqqg\rangle + |qqqu\bar{u}\rangle + |qqqd\bar{d}\rangle + |qqqs\bar{s}\rangle + |qqqgg\rangle$$

$|qqq\ gg\rangle \sim$ 6 color singlet state

1 singlet $\otimes$ singlet

4 octet $\otimes$ octet

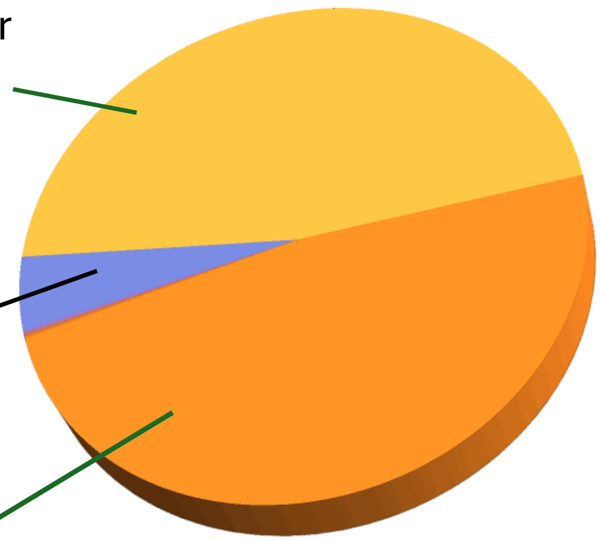
1 decuplet $\otimes$ octet $\otimes$ octet

$|qqq\ ggg\rangle \sim$ 22 color singlet state

2 singlet $\otimes$ singlet

16 octet $\otimes$ octet

4 decuplet $\otimes$ octet $\otimes$ octet $\otimes$ octet



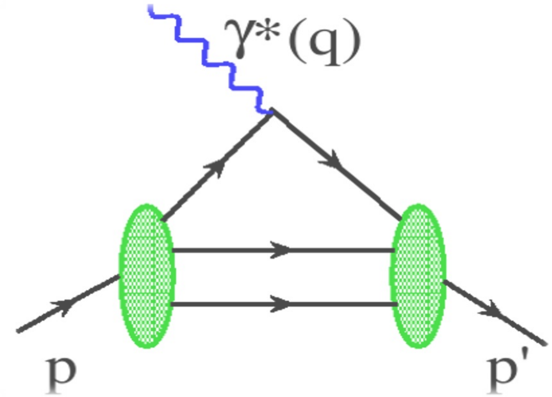
m_u	m_d	m_s	m_f	g	b	b_{inst}
0.5 GeV	0.40 GeV	0.6 GeV	2.5 GeV	2.0	0.6 GeV	3.0 GeV

Truncation parameter: $N_{\max} = 7$ and $K_{\max} = 10$

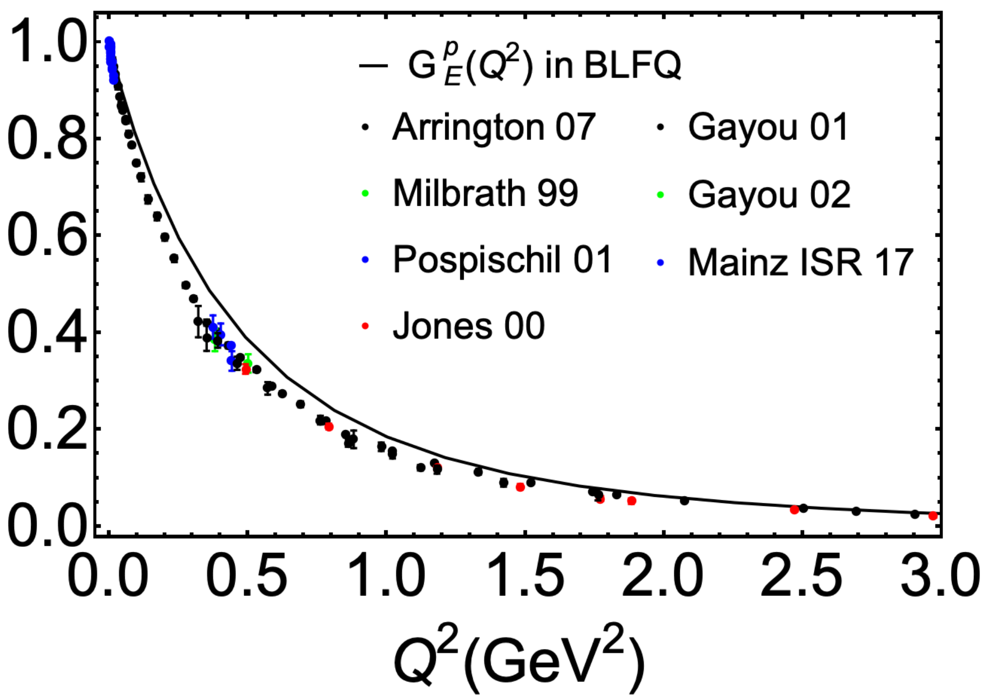
Nucleon Form Factors

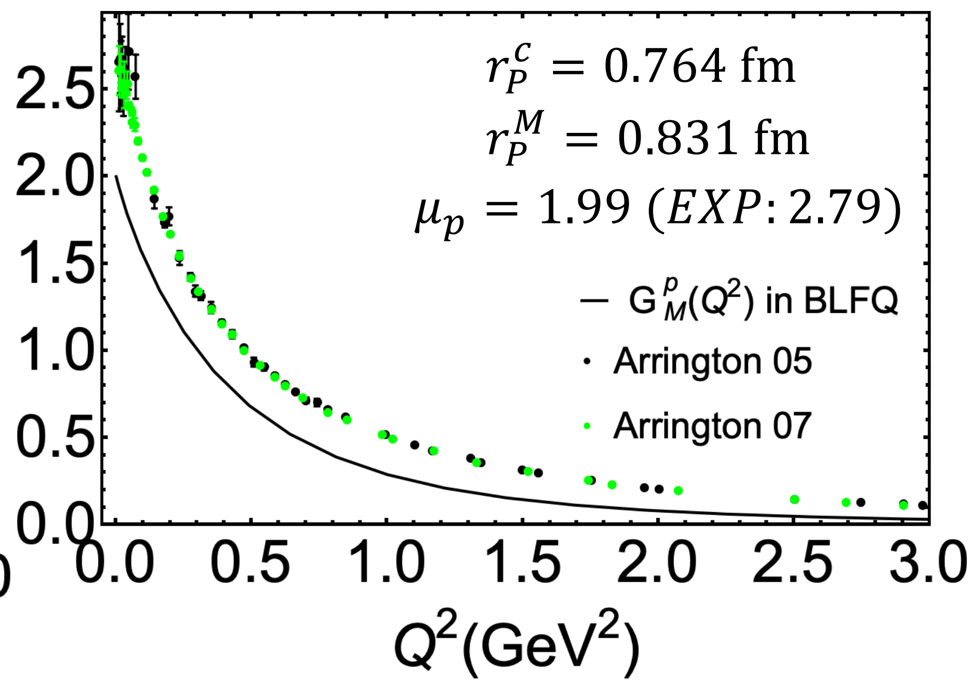
$$\langle N(p')|J^{\mu}(0)|N(p)\rangle =$$

$$\bar{u}(p')\left[\gamma^{\mu}\underbrace{F_1(q^2)} + \frac{i\sigma^{\mu\nu}}{2m_N}q_{\nu}\underbrace{F_2(q^2)}\right]u(p)$$



Preliminary results





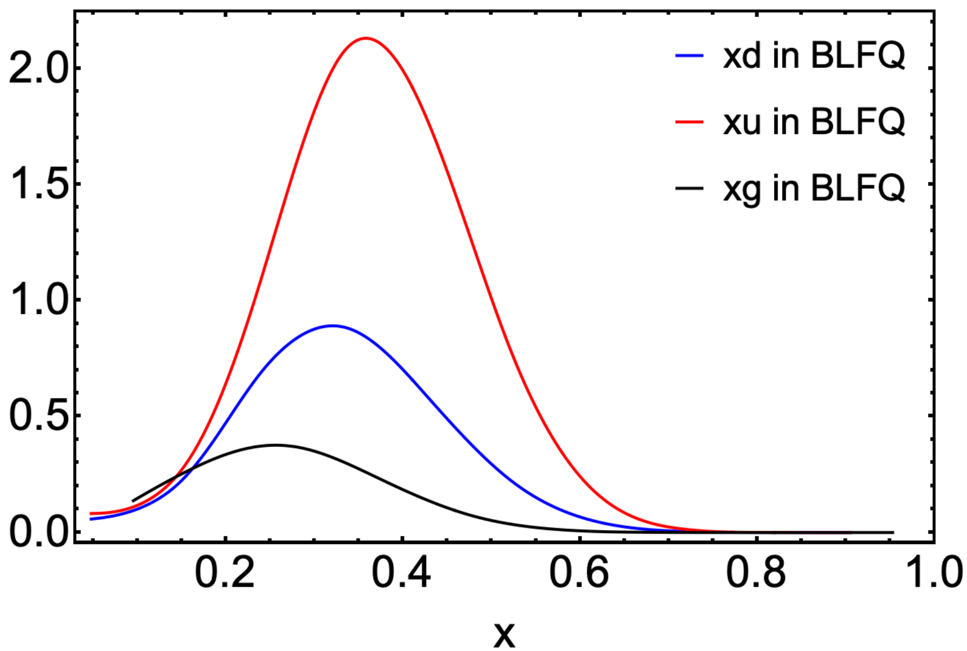
- BLFQ results qualitatively agree with the experimental data for Dirac and Pauli FFs

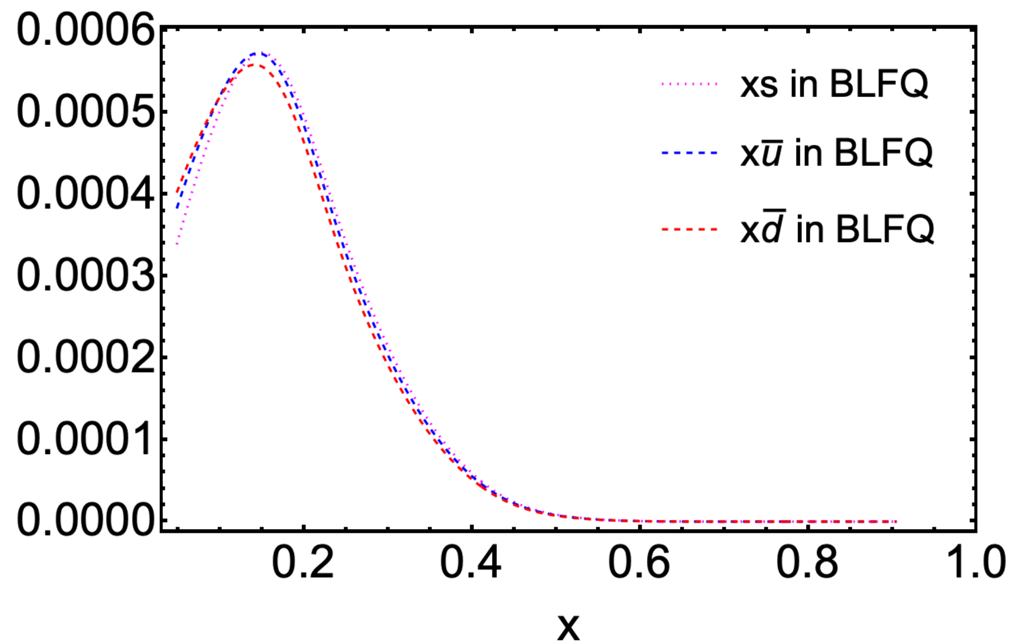
Unpolarized Parton Distribution Function

- Parton distribution functions with five Fock sectors
  - Qualitative behavior agree with experimental results
  - Endpoint behavior improves with $|qqqgg\rangle$ and $|qqqggg\rangle$ Fock sector included
  - Five-particle sector contributions are small due to Fock sector truncation (no $|qqq\ q\bar{q}\ g\rangle$),

Preliminary results

All results at the initial scale



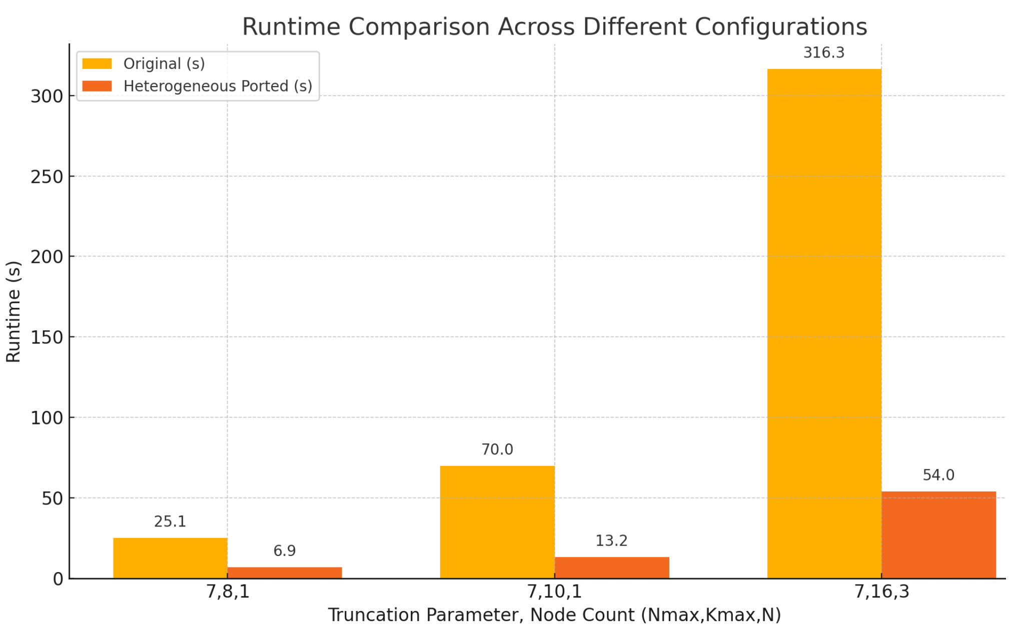


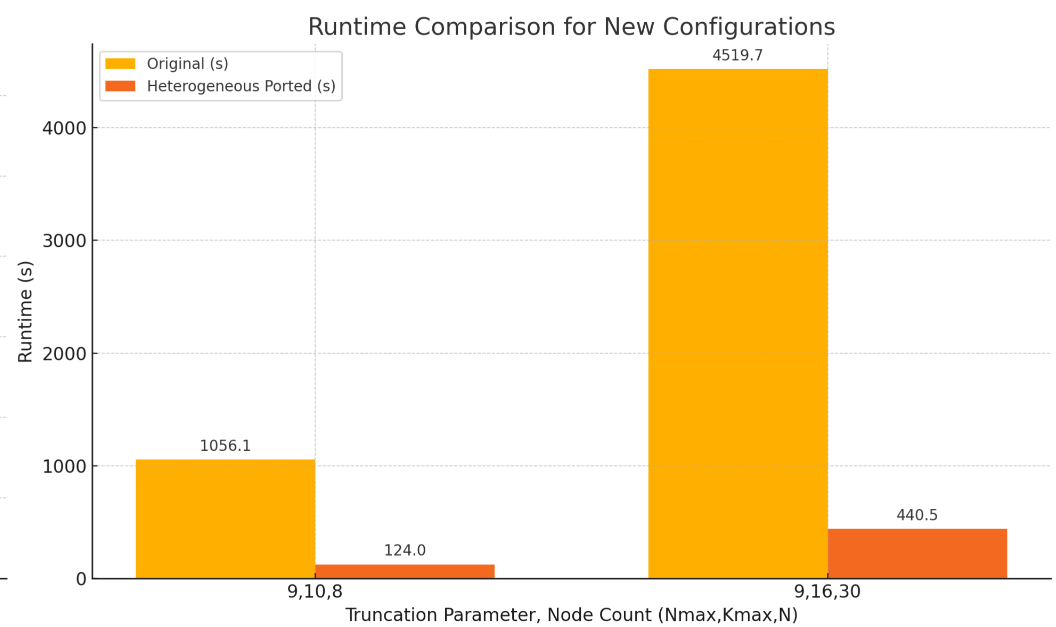
BLFQ Optimization - Diagonalization

Diagonalization: Arpack

Replace the Basic function
BLAS -> HIPBLAS
LAPACK -> GPU Adaptation

Reprogram the Kernel:
Arpack Kernel, Matrix Multiplication



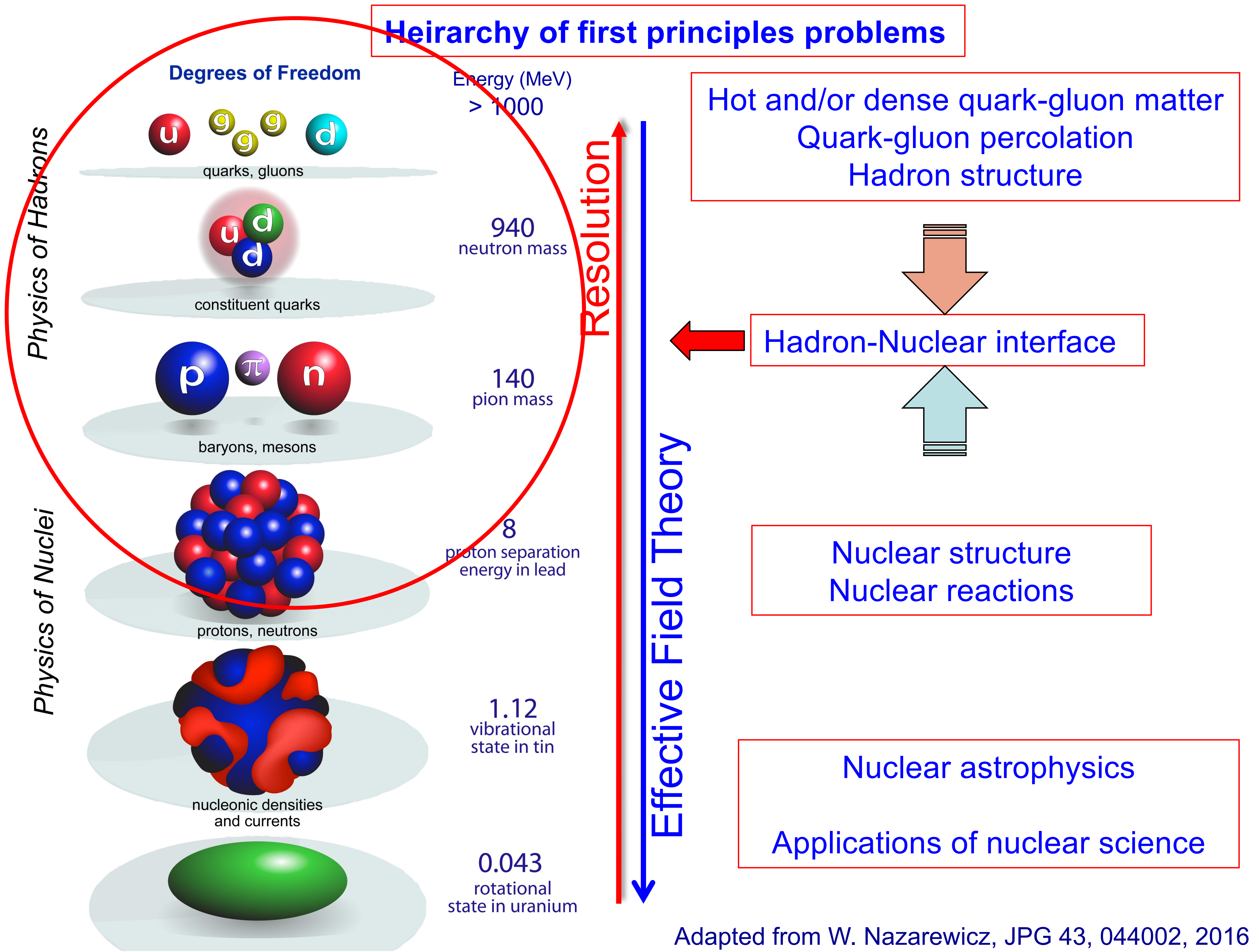


Sample of next steps for BLFQ & tBLFQ

- Improve the BLFQ basis to include chiral symmetry breaking
  Y. Li and J.P. Vary, Phys. Letts. B 825, 136860 (2022)
  Y. Li, P. Maris and J.P. Vary, Phys. Letts. B 836, 137598 (2023)
- Increase the number of dynamical gluons
- Include sea quark pairs
- Address the proton spin puzzle
- Investigate exotic systems: glueballs, tetraquarks, pentaquarks, . . .
- Calculate meson-meson, meson-baryon and baryon-baryon interactions
- Predict the six-quark cluster structure contributions to nuclear properties such as the EMC effect and $x > 1$ physics

. . .

Now turn our attention to Chiral EFT
theory of inter-nucleon interactions with origins in QCD



Heirarchy of first principles problems
Degrees of Freedom
Energy (MeV)
> 1000
u
g
g
g
d
quarks, gluons
u
d
d
constituent quarks
940
neutron mass
p
π
n
baryons, mesons
140
pion mass
8
proton separation
energy in lead
protons, neutrons
1.12
vibrational
state in tin
nucleonic densities
and currents
0.043
rotational
state in uranium
Physics of Hadrons
Physics of Nuclei
Resolution
Effective Field Theory
Hot and/or dense quark-gluon matter
Quark-gluon percolation
Hadron structure
Hadron-Nuclear interface
Nuclear structure
Nuclear reactions
Nuclear astrophysics
Applications of nuclear science
Adapted from W. Nazarewicz, JPG 43, 044002, 2016

An Effective Field Theory (EFT) expresses a system's properties in terms of the constituents (degrees of freedom) most relevant to the energy/momentum scales being probed. An EFT is derivable, in principle, from an underlying theory such as the Standard Model.

For the low-lying spectroscopy and reactions of the mesons and baryons, this could be an EFT of interacting constituent quarks and gluons.
Example: Basis Light Front Quantization (BLFQ) with Effective Hamiltonians inspired by Light-Front Holography with residual interactions from QCD.

For the low-lying spectroscopy and reactions of atomic nuclei this could be Chiral EFT applied within the *ab initio* No-Core Shell Model (NCSM)

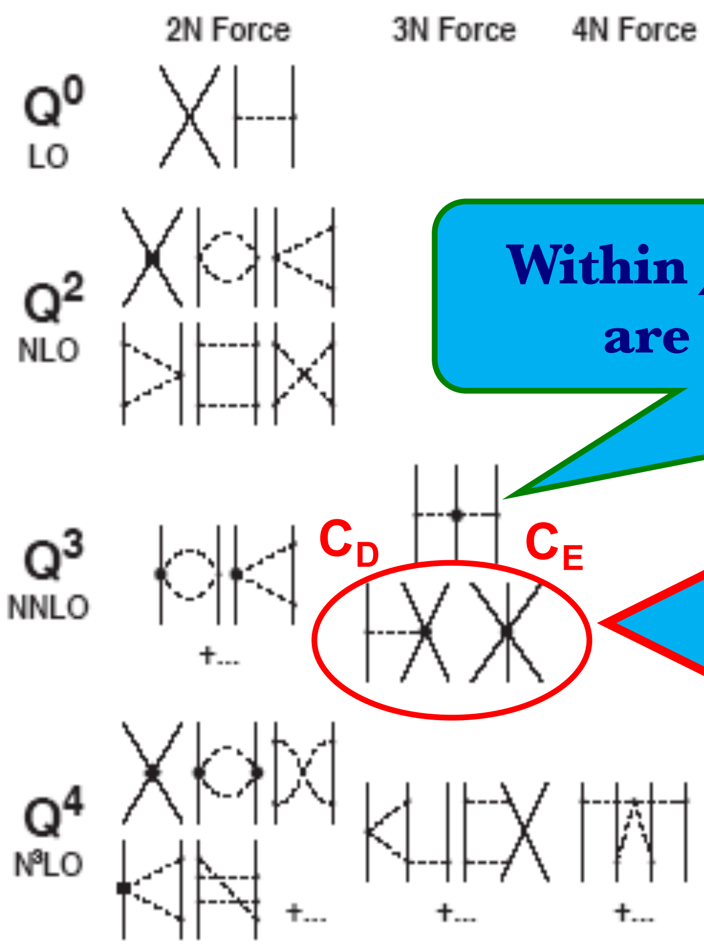
Effective Nucleon Interaction

Chiral Perturbation Theory (χPT)

Weinberg's χPT allows for controlled power series expansion

$$\text{Expansion parameter}: \left(\frac{Q}{\Lambda_\chi}\right)^{\upsilon},\ Q - \text{momentum transfer},$$

$$\Lambda_\chi \approx 1\ GeV,\ \chi\text{ - symmetry breaking scale}$$



Within χPT 2π-NNN Low Energy Constants (LEC) are related to the NN-interaction LECs $\{c_i\}$

Additional terms from χPT with LECs specific to NNN systems

Regularization is essential, which is also implicit within the Harmonic Oscillator (HO) wave function basis (see below)

R. Machleidt and D.R. Entem, Phys. Rep. 503, 1 (2011);
E. Epelbaum, H. Krebs, U.-G Meissner, Eur. Phys. J. A51, 53 (2015); Phys. Rev. Lett. 115, 122301 (2015)

Adapted from P. Navratil slide

No Core Shell Model (NCSM)
A large sparse matrix eigenvalue problem

$$H = T_{rel} + V_{NN} + V_{3N} + \bullet\bullet\bullet$$
$$H\left|\Psi_i\right\rangle = E_i\left|\Psi_i\right\rangle$$
$$\left|\Psi_i\right\rangle = \sum_{n=0}^{\infty} A_n^i \left|\Phi_n\right\rangle$$
$$\text{Diagonalize } \left\{\left\langle\Phi_m\right|H\left|\Phi_n\right\rangle\right\}$$

P. Navratil, J. P. Vary and B.R. Barrett, *Phys. Rev. Lett.* **84**, 5728 (2000); *Phys. Rev. C* **62**, 054311 (2000)

- Adopt realistic NN (and NNN) interaction(s) & renormalize as needed - retain induced many-body interactions: Chiral Effective Field Theory (Chiral EFT) interactions
- 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 (each determinant manages the bookkeeping of anti-symmetrization)
- Diagonalize this sparse many-body H in its "m-scheme" basis where [$\alpha = (n,l,j,m_j,\tau_z)$]

HO basis space (configurations)

$$\left\{ \begin{array}{l} \left|\Phi_n\right\rangle = [a_\alpha^+ \bullet\bullet\bullet a_\varsigma^+]_n \left|0\right\rangle \\ n = 1,2,\ldots,10^{10} \text{ or more!} \end{array} \right.$$

- Evaluate observables and compare with experiment

Comments

- Computationally demanding => needs new algorithms & high-performance computers
- Requires convergence assessments and extrapolation tools to retain predictive power
- Achievable for nuclei up to atomic number of about 20 with largest computers available

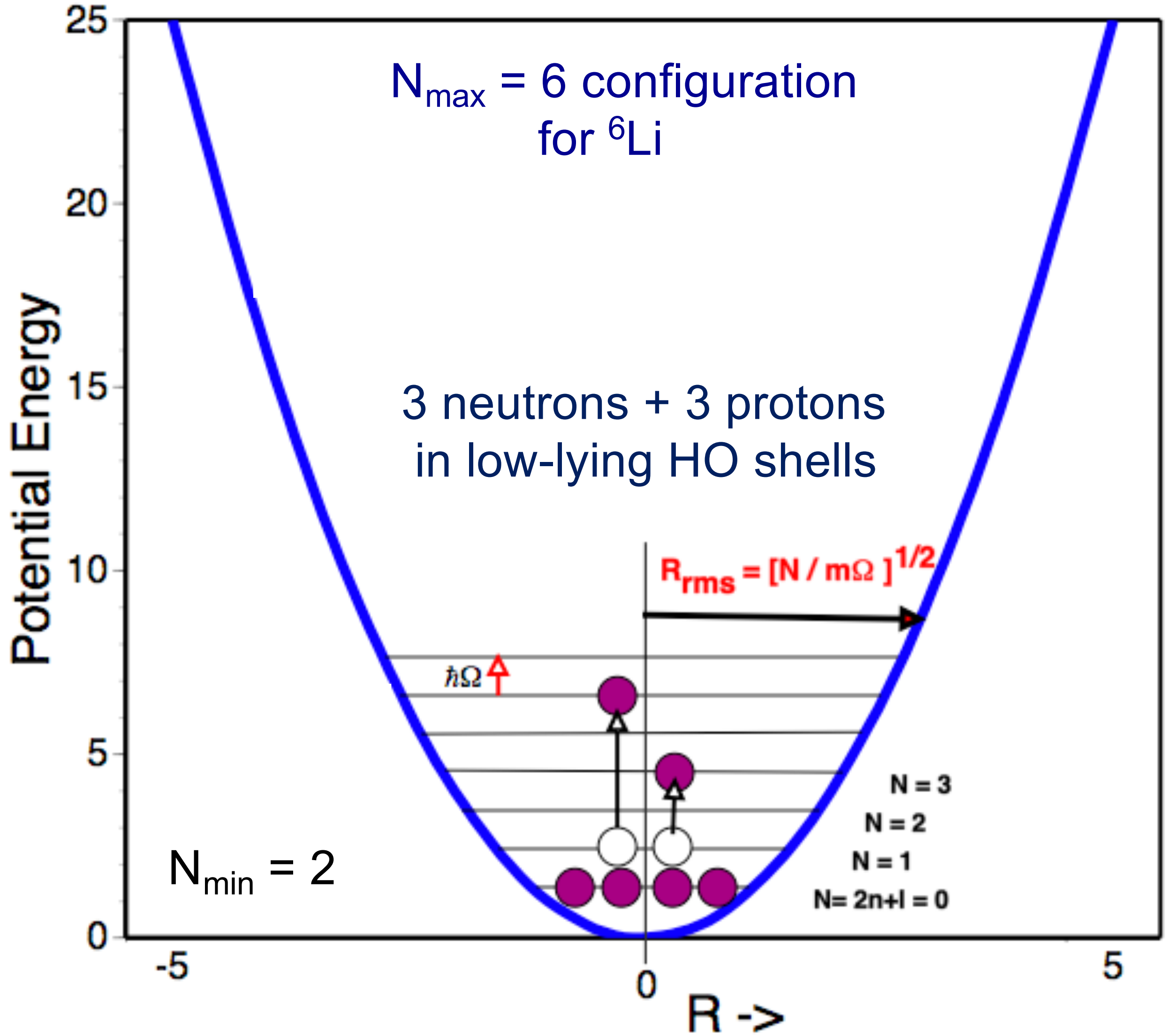
$N_{\min} \equiv$ HO quanta of lowest configuration

$N_{\max} \equiv$ maximum HO quanta above the lowest configuration

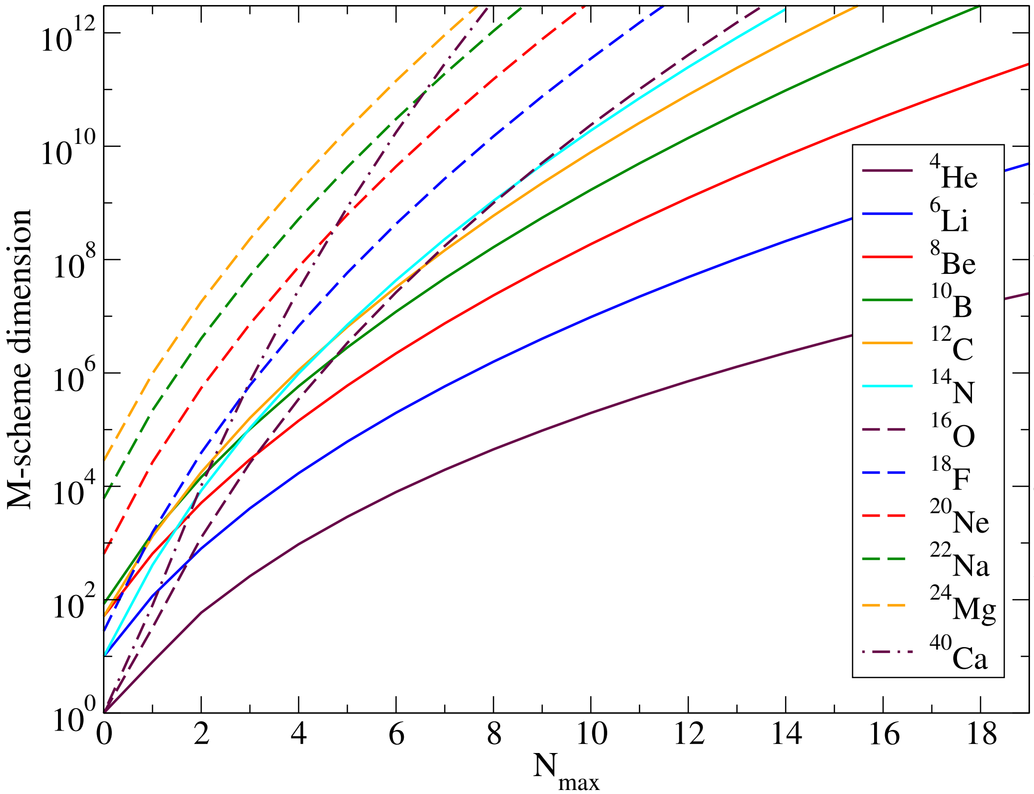
Retain configurations with $N_{\min} \leq \sum_{i=1}^{A}(2n_i + l_i) \leq N_{\min} + N_{\max}$

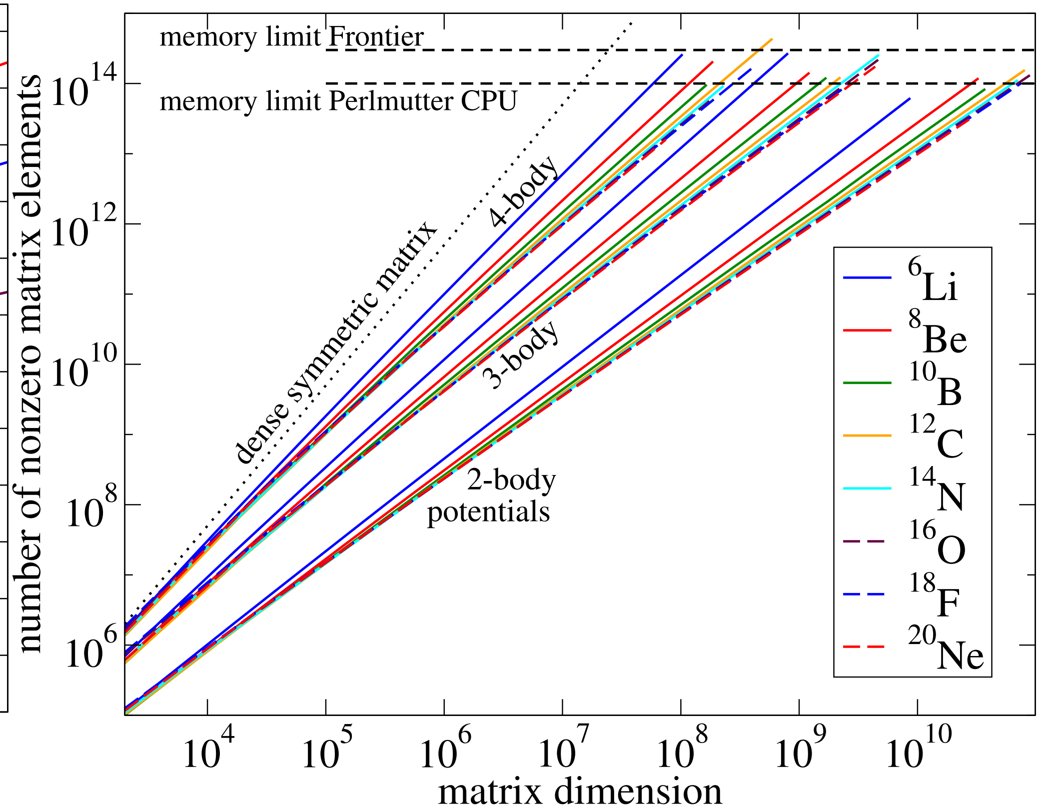
consistent with symmetry constraints (parity, M_J,...)

extrapolate: N_{max} -> infinity



Challenge
Exponential increase in Matrix Dimension (D)





Opportunities

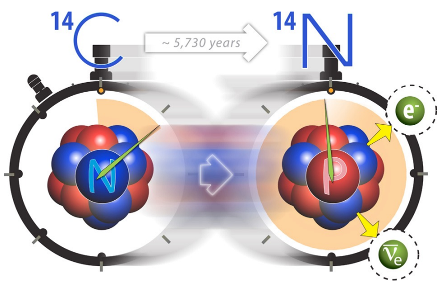
- Memory/cpu time grows only as $D^{3/2}$
- Algorithm development (SciDAC funding)
- Exaflop machines now available (DOE/INCITE competitive awards)
- Improved understanding of Chiral EFT
- Developing methods for extrapolating D->inf (N_{max}->inf)

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]

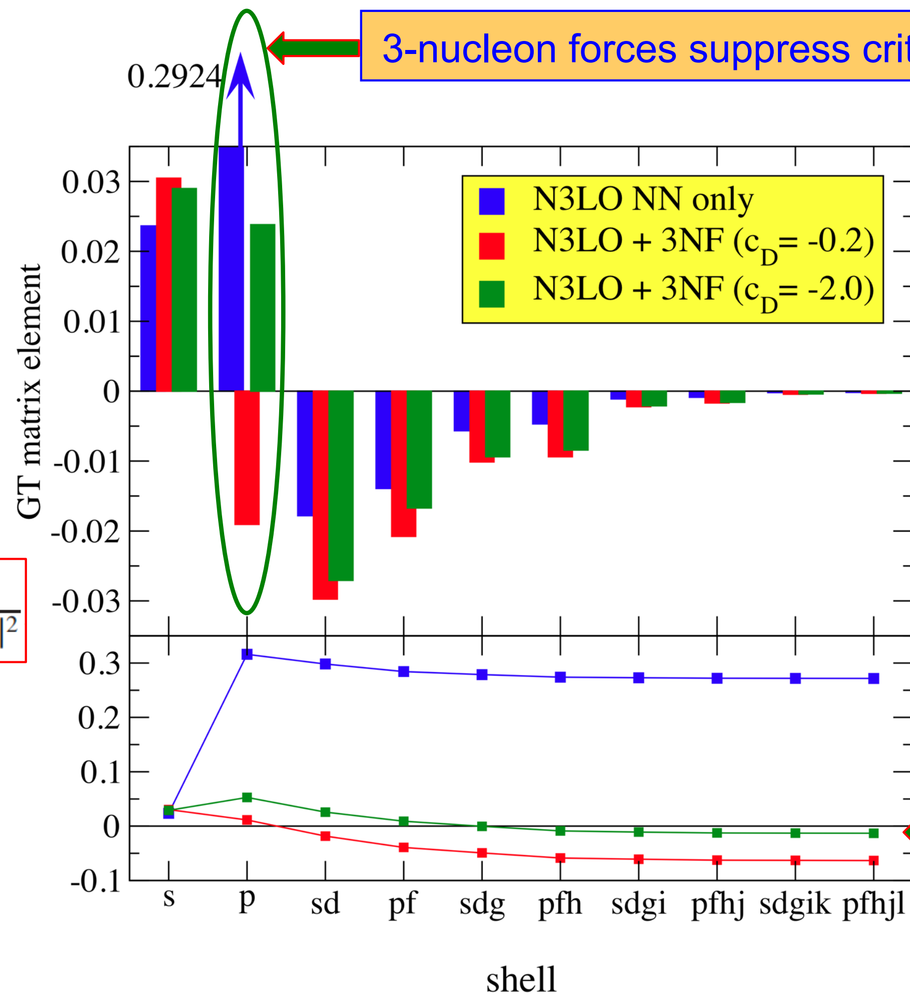
- Solves the puzzle of the long but useful lifetime of ^{14}C
- Establishes a major role for strong 3-nucleon forces in nuclei
- Strengthens foundation for guiding experiments



$$T_{1/2} = \frac{1}{f(Z,E_0)} \frac{2\pi^3\hbar^7 \ln 2}{m_e^5 c^4 G_V^2} \frac{1}{g_A^2 |M_{GT}|^2}$$

$$M_{GT} = \sum_k \langle \Psi_f || \sigma(k)\tau_+(k) || \Psi_i \rangle$$

3-nucleon forces suppress critical component



net decay rate
Is very small

- Dimension of matrix solved for 8 lowest states ~ 1×10^9
- Each run 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)

PHYSICAL REVIEW C **103**, 054001 (2021)

Editors' Suggestion

Light nuclei with semilocal momentum-space regularized chiral interactions up to third order

P. Maris,[1,*] E. Epelbaum,[2] R. J. Furnstahl,[3] J. Golak,[4] K. Hebeler,[5,6] T. Hüther,[5] H. Kamada,[7] H. Krebs,[2] Ulf-G. Meißner,[8,9,10] J. A. Melendez,[3] A. Nogga,[9] P. Reinert,[2] R. Roth,[5] R. Skibiński,[4] V. Soloviov,[4] K. Topolnicki,[4] J. P. Vary,[1] Yu. Volkotrub,[4] H. Witała,[4] and T. Wolfgruber[5]

The LENPIC team:
www.lenpic.org

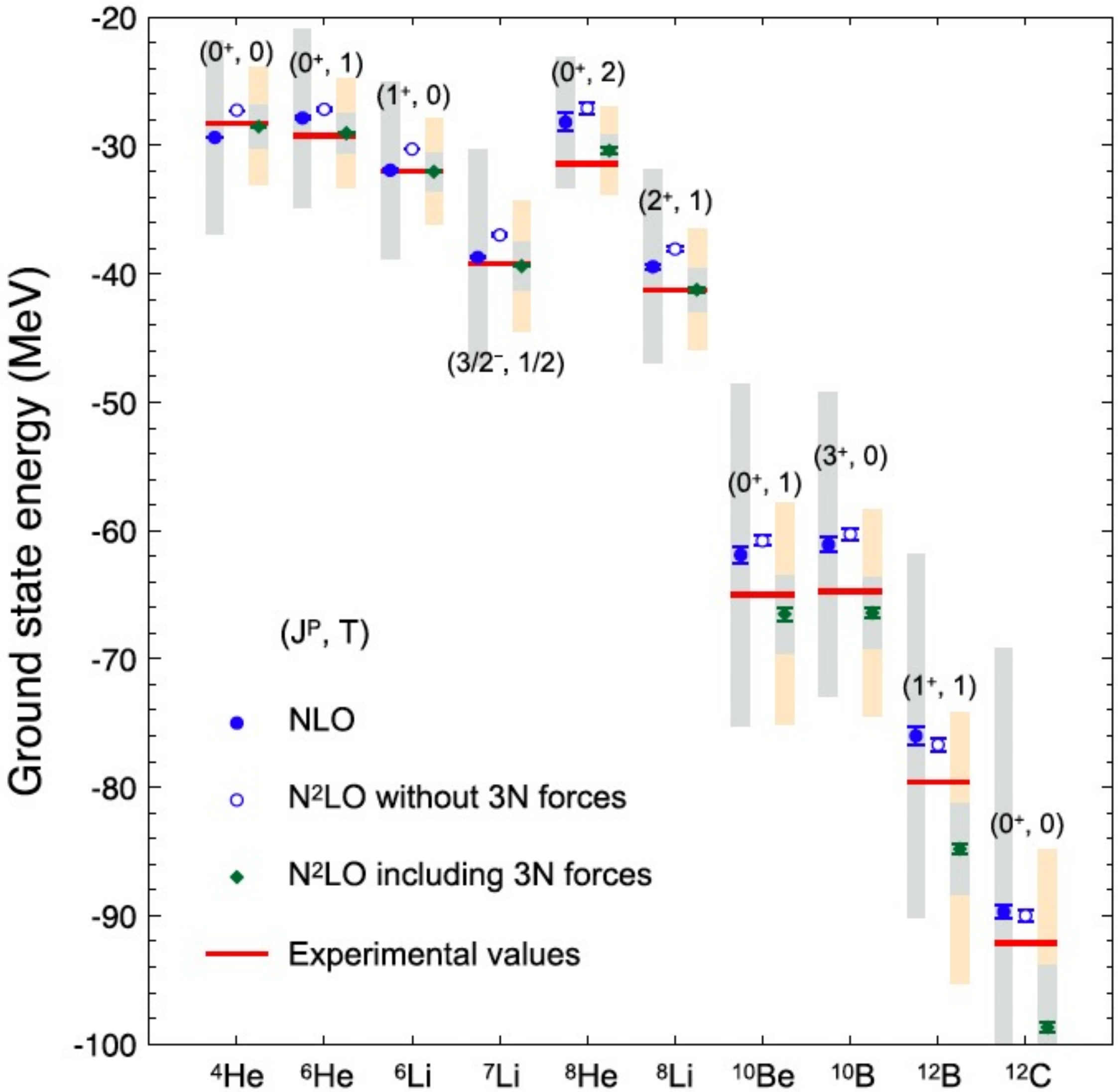


FIG. 8. Calculated ground-state energies in MeV using chiral NLO, and N^2LO interactions at $\Lambda = 450$ MeV (blue and green symbols) in comparison with experimental values (red levels). For each nucleus the NLO, and N^2LO results are the left and right symbols and bars, respectively. The open blue symbols correspond to incomplete calculations at N^2LO using NN-only interactions. Blue and green error bars indicate the NCCI extrapolation uncertainty. All results shown are for $\alpha = 0.08$ fm^4. The light (coral) and dark (gray) shaded bars indicate the 95% and 68% DoB truncation errors, respectively, estimated using the Bayesian model $\bar{C}^{650}_{0.5-10}$ (at NLO we only show the 68% DoB truncation errors because the 95% errors would be off one or even both ends of the scale).

Excitation energies from effective field theory with quantified uncertainties

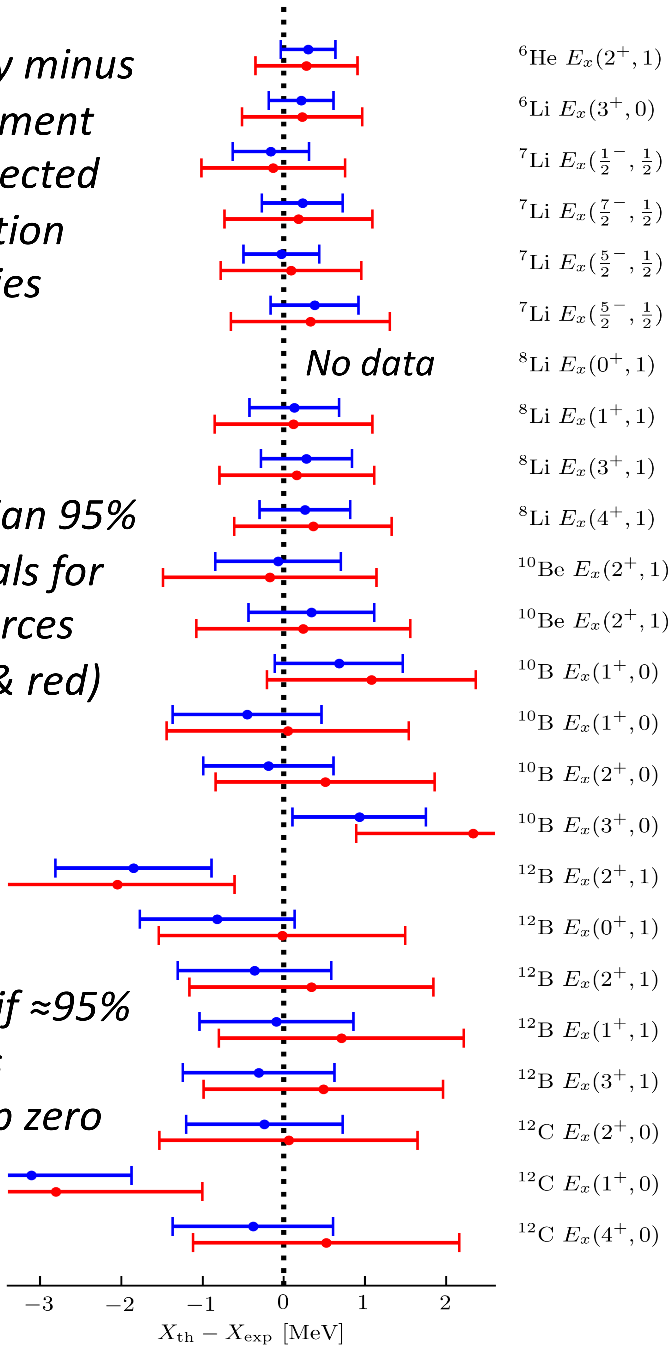
U.S. DEPARTMENT OF ENERGY | Office of Science

NUCLEI — Nuclear Computational Low-Energy Initiative

Theory minus experiment for selected excitation energies

Bayesian 95% intervals for two forces (blue & red)

Check if ≈95% of bars overlap zero



Objectives

- Predict properties of ground and excited states of light nuclei with robust theoretical error estimates.
- Test consistent LENPIC chiral effective field theory (EFT) interactions with 2- and 3-nucleon forces.
- Extend and test a Bayesian statistical model that learns from the order-by-order EFT convergence pattern to account for correlated excitations.

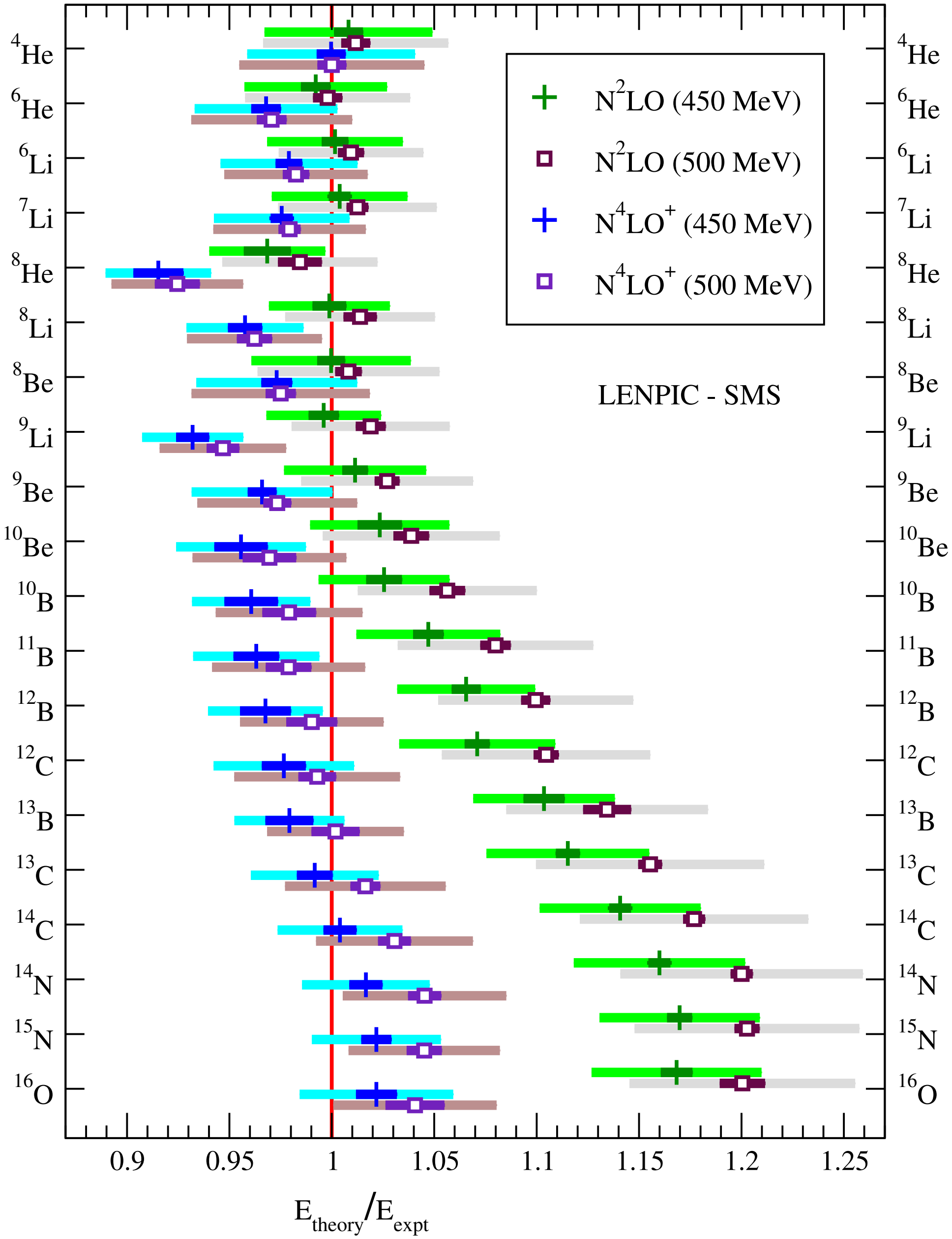
Impact

- First test of novel chiral nucleon-nucleon potentials with consistent three-nucleon forces.
- Demonstrates understanding of theoretical uncertainties due to chiral EFT expansion.
- Accounting for correlations produces agreement with experimental excitation energies (see figure).
- Exceptions in ^{12}C and ^{12}B indicate different theoretical correlations in the nuclear structure.

Accomplishments

P. Maris et al, Phys. Rev. C **103**, 054001 (2021); Editors' Suggestion; arXiv: 2012.12396 [nucl-th]

Binding Energies with LENPIC-SMS chiral EFT



P. Maris, H. Le, A. Nogga, R. Roth, J.P. Vary
Front. Phys. 11, 1098262 (2023)

- NN potential up to N^{4}LO$^+$
- 3NFs at N^{2}LO
- SRG evolved to $\alpha = 0.08$ fm^4
- LECs fitted to
  - NN scattering data
  - ^{3}H binding energy
  - Nd scattering
- Parameter-free predictions
- Error bars
  - numerical uncertainty
  - chiral EFT uncertainty from Bayesian analysis

Adapted from P. Maris, LENPIC Annual Meeting, Bonn, March 11-13, 2024

Daejeon16 NN interaction

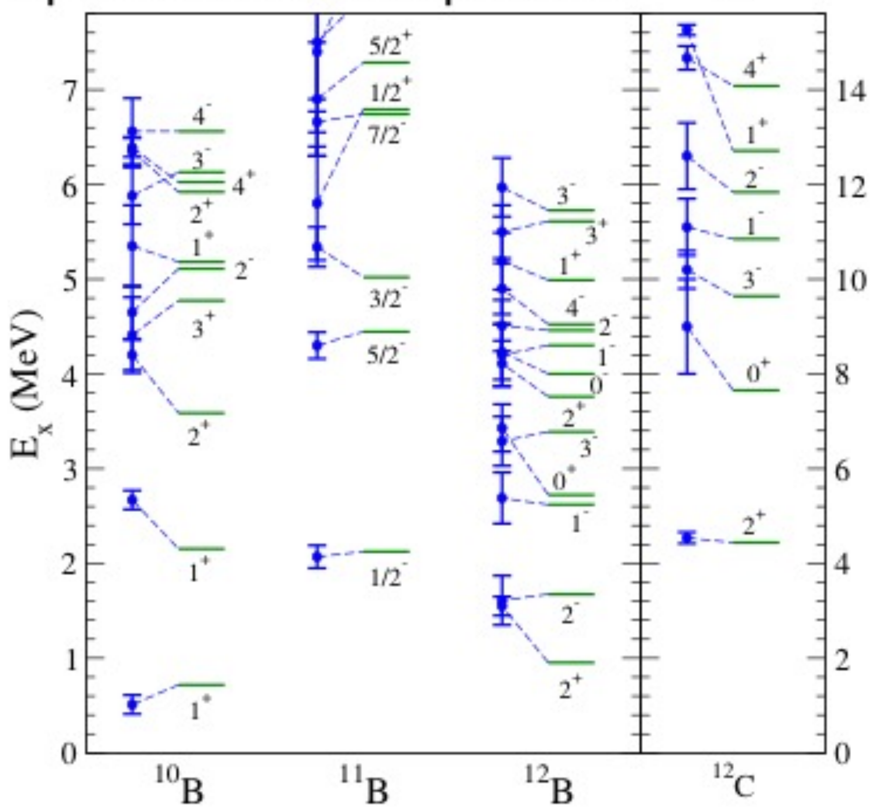
Based on SRG evolution of Entem-Machleidt “500” chiral N3LO to $\lambda = 1.5\ \mathrm{fm}^{-1}$ followed by Phase-Equivalent Transformations (PETs) to fit selected properties of light nuclei.

A.M. Shirokov, I.J. Shin, Y. Kim, M. Sosonkina, P. Maris and J.P. Vary, “N3LO NN interaction adjusted to light nuclei in ab exitu approach,” Phys. Letts. B 761, 87 (2016); arXiv: 1605.00413

Application to excited states of p-shell nuclei

(Maris, Shin, Vary, in preparation)

Spectra of B isotopes and ^{12}C



- difference of extrapolated E_b
- extrapolation uncertainties: max of E_b uncertainties
- good agreement with positive and negative parity spectra
- need large bases for ’intruder’ and ’non-normal parity’ states
- spectrum ^{10}B
  - correct gs 3^+ and excited 1^+
  - third 1^+ ’intruder’ state
- excited 0^+ state in ^{12}C
  - Hoyle state?
  - see MCNCSM results below

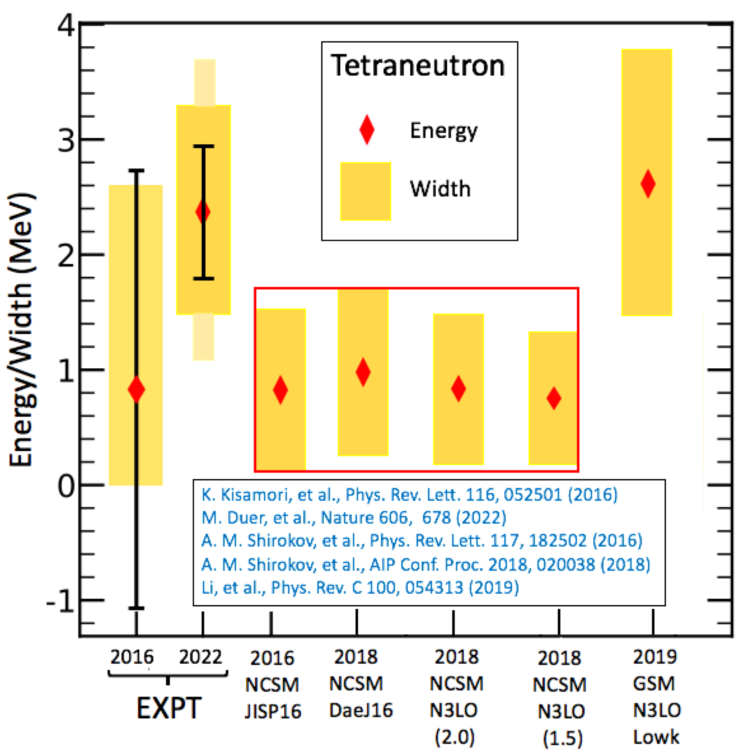
Tetraneutron discovery confirms prediction

U.S. DEPARTMENT OF ENERGY | Office of Science

NUCLEI — Nuclear Computational Low-Energy Initiative

Objectives

- *Ab initio* nuclear theory aims for parameter-free predictions of nuclear properties with controlled uncertainties using supercomputer simulations
- Specific goal is to predict if the tetraneutron (4-neutron system) has a bound state, a low-lying resonance or neither



Experiment and theory for the tetraneutron's resonance energy and width. *Ab initio* No-Core Shell Model (NCSM) and Gamow Shell Model (GSM) predictions use different neutron-neutron interactions and different basis function techniques.

Impact

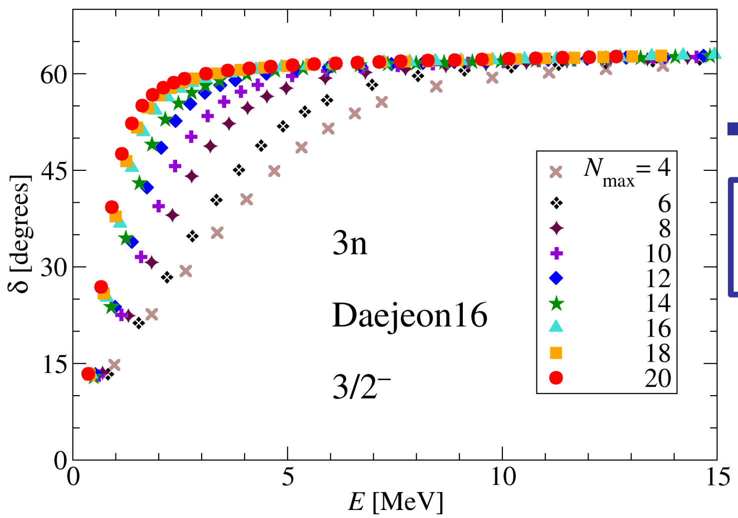
- Discovery in 2022 announced in Nature [1] confirms *ab initio* theory predictions from 2016 [2] of a short-lived tetraneutron resonance at low energy and the absence of a tetraneutron bound state
- Demonstrates the predictive power of *ab initio* nuclear theory since theory and experiment are within their combined uncertainties
- Sets stage for further experimental and theoretical research on new states of matter formed only of neutrons
- Shows need to anticipate a long wait time for experimental confirmation of such an exotic phenomena, ~ 6 years in this case
- Emphasizes the value of DOE supercomputer allocations (NERSC) and support for multi-disciplinary teamwork (SciDAC/NUCLEI)

Accomplishments

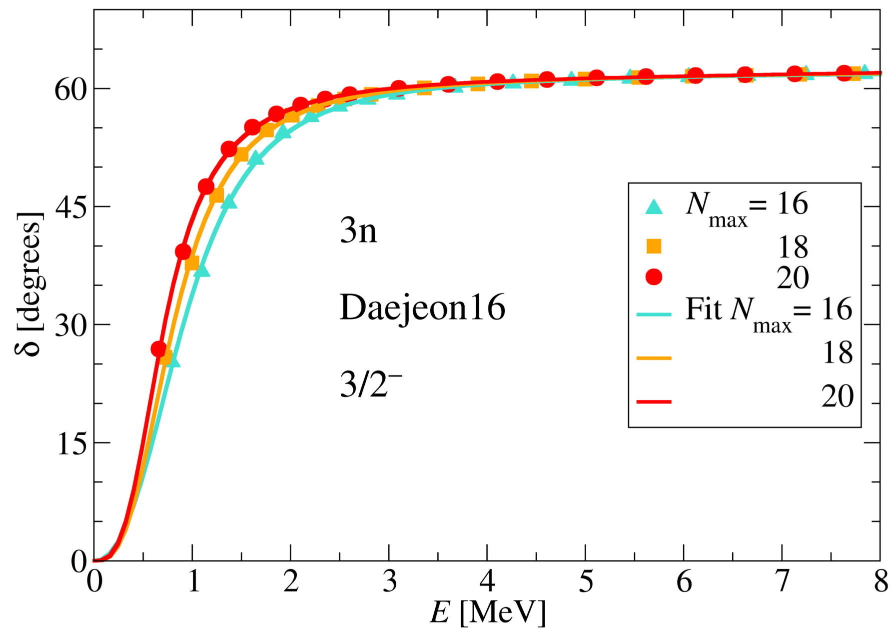
[1] M. Duer, et al., Nature 606, 678 (2022)

[2] A.M. Shirokov, G. Papadimitriou, A.I. Mazur, I.A. Mazur, R. Roth and J.P. Vary, "Prediction for a four-neutron resonance," Phys. Rev. Lett. 117, 182502 (2016)

3n Results with Daejeon16 NN interaction



Selection of points, parameterization



Extraction of S-matrix pole position

N_{max}	$3/2^-$		$1/2^-$	
	E_r [MeV]	Γ [MeV]	E_r [MeV]	Γ [MeV]
16	0.607	1.524	0.606	1.604
18	0.537	1.176	0.531	1.133
20	0.481	0.963	0.481	0.962

I.A. Mazur, M. K. Efimenko, A. I. Mazur, I. J. Shin, V. A. Kulikov, A. M. Shirokov and J. P. Vary, Rev. C 110, 014004 (2024); arXiv: 2403.18232

Alpha clusters in Carbon-12 from ab initio theory & statistical learning

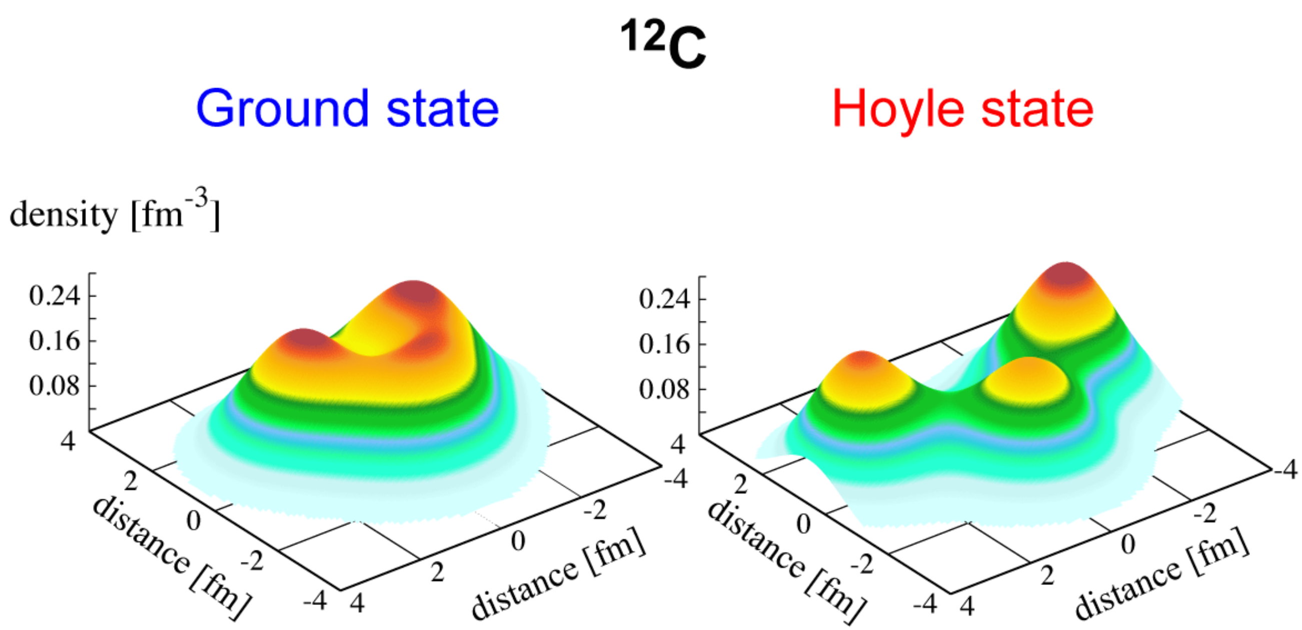
Objectives

- *Ab initio* nuclear theory aims for parameter-free predictions of critical nuclear properties with controlled uncertainties using supercomputer simulations
- Specfic goal is to determine extent of alpha clustering in the Ground state and the Hoyle state of Carbon-12 (^{12}C)

Impact

- Ground state found to have 6% alpha clustering while Hoyle state discovered to be 3-alphas 61% of the time
- With this high percentage of 3-alphas, the Hoyle state is confirmed as a natural gateway state for the cosmic formation of ^{12}C, the key element for organic life
- Statistical learning confirms 3-alpha feature of Hoyle state

Ab initio Monte-Carlo Shell Model results for density contours of 12C Ground state and first excited 0^+ (Hoyle) state using the Daejeon16 two-nucleon potential. Simulations were performed on Fugaku in Japan, the world's largest supercomputer at the time.

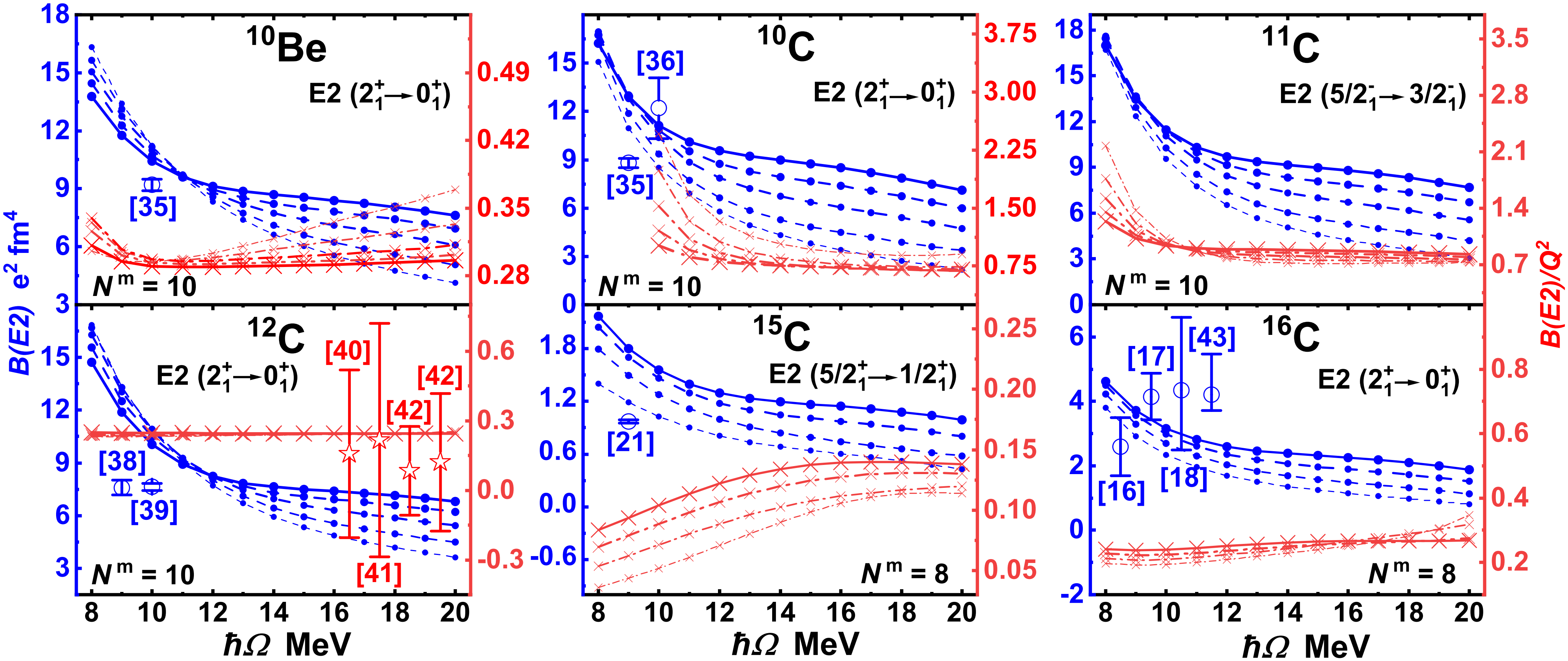


Accomplishments

T. Otsuka, T. Abe, T. Yoshida, Y. Tsunoda, N. Shimizu, N. Itagaki, Y. Utsuno, J. Vary, P. Maris and H. Ueno, "Alpha-Clustering in Atomic Nuclei from First Principles with Statistical Learning and the Hoyle State Character," Nature Communications 13:2234 (2022)

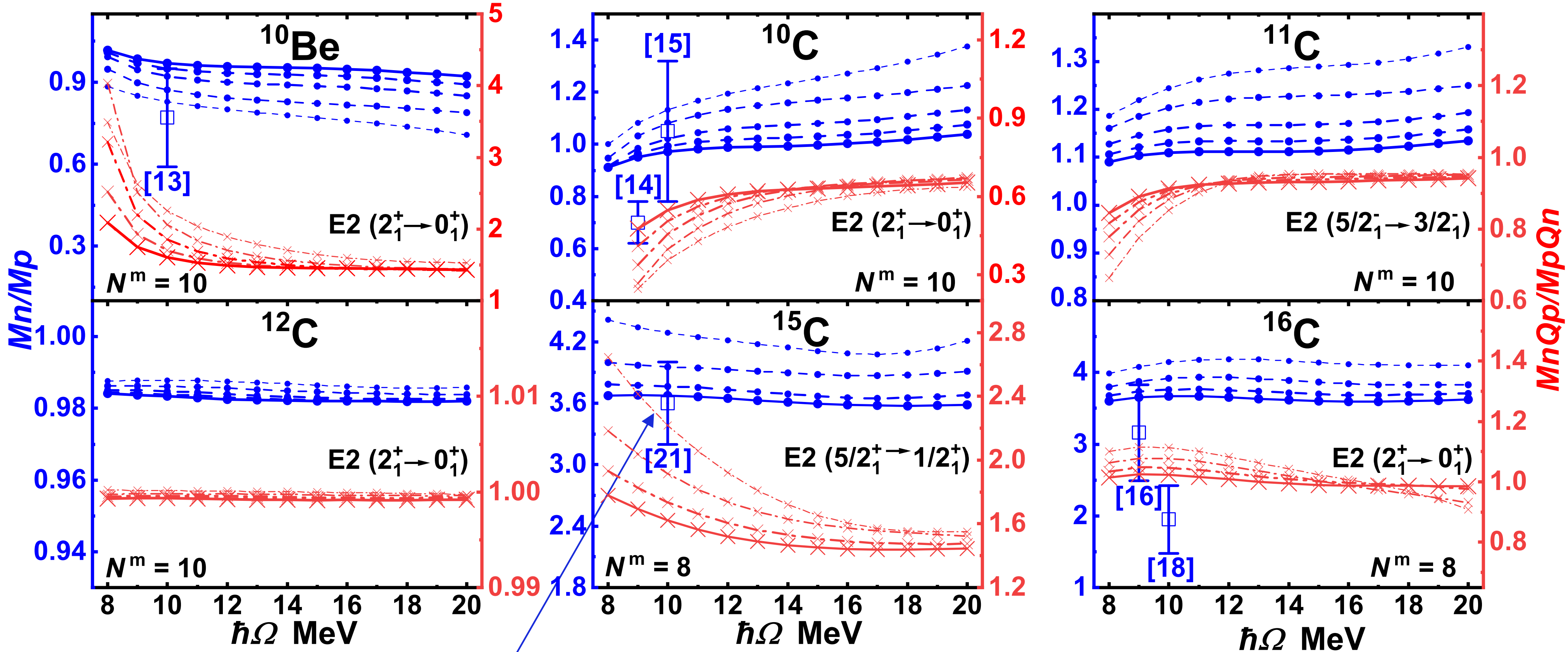
$$\frac{B(E2)}{Q_p^2} = \frac{\langle J_f || \sum_{i\in p} r_i^2 Y_2(\hat{r}_i) || J_i \rangle^2}{\langle J_i || \sum_{i\in p} r_i^2 Y_2(\hat{r}_i) || J_i \rangle^2},$$

Ratios of observables converge better
He Li, et al., arXiv: 2401.05776



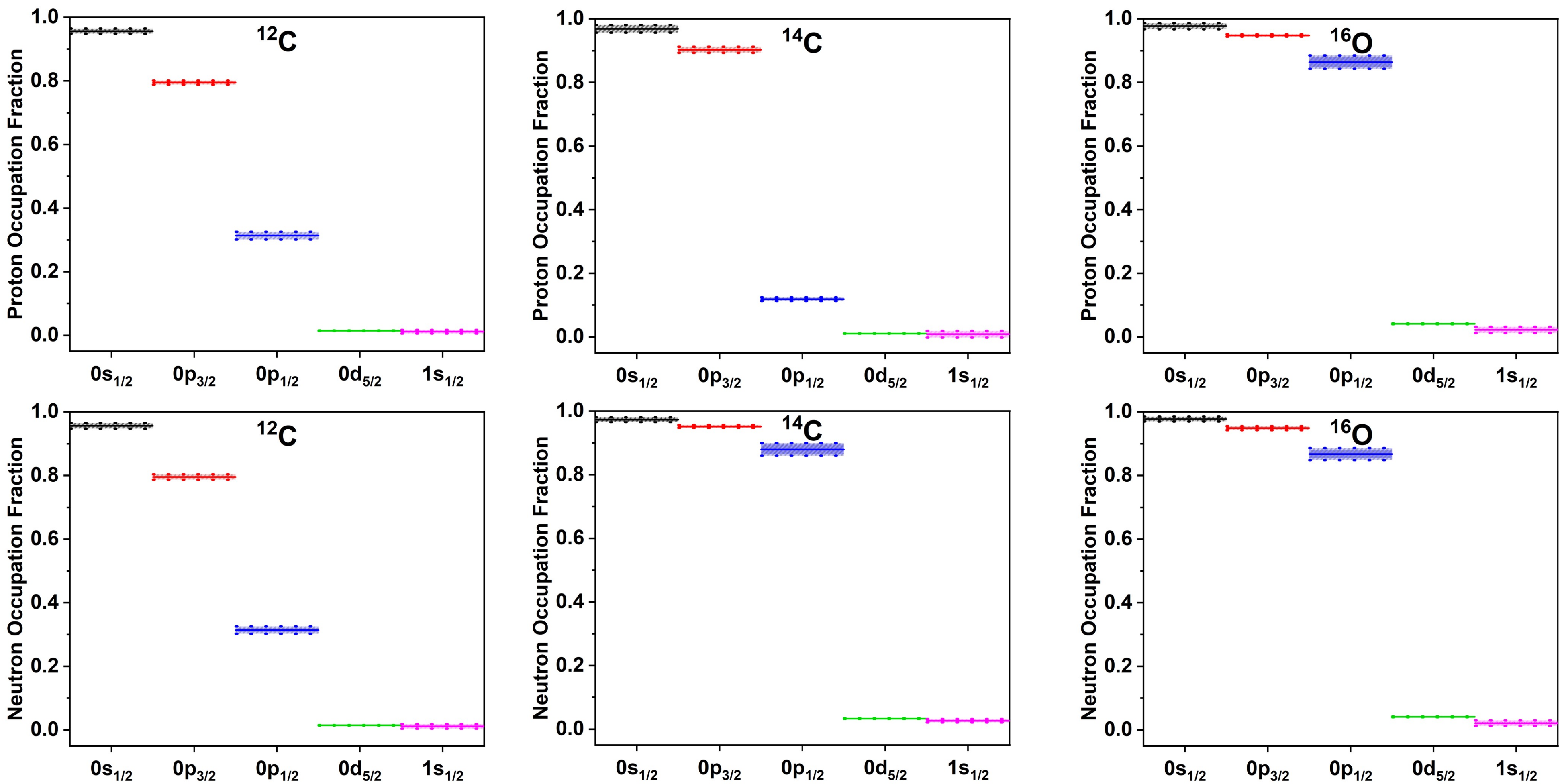
$$\frac{M_n}{M_p} = \frac{\langle J_f || \sum_{i\in n} r_i^2 Y_2(\hat{r}_i) || J_i\rangle}{\langle J_f || \sum_{i\in p} r_i^2 Y_2(\hat{r}_i) || J_i\rangle},$$

Ratios of observables and ratios of ratios converge better
He Li, et al., arXiv: 2401.0577



Jie Chen et al., PRC 106, 064312 (2022)

Z = 6 show good subshell closure at N = 8 (i.e. “locally magic”)



Ground state occupation fractions of protons (neutrons) in low-lying single particle states in ^{12}C, ^{14}C, and ^{16}O. The NCSM calculations performed in a harmonic oscillator basis using the Daejeon16 *NN* interaction with N_{max} = 10 and $\hbar\Omega$ = 17.5 MeV. We present uncertainties where the lowest (highest) point indicates the minimal (maximal) occupation fraction value in the range from $\hbar\Omega$ = 15 to 20 MeV.

H. Li, H.J. Ong, Dong-Liang Fang, I.A. Mazur, I.J. Shin, A.M. Shirokov, J.P. Vary, Peng Yin, Xing-Bo Zhao and Wei Zuo, Chinese Physics C 48, 124103 (2024); arXiv: 2407.09734

What lies ahead for nuclear theory across energy scales?

- Need for increased theory effort at deriving and validating EFTs
  Expand multi-disciplinary and multi-national collaborative efforts

- Need for enhanced computational power to greatly expand basis spaces
  Artificial Intelligence and/or Quantum Computing can be keys to progress

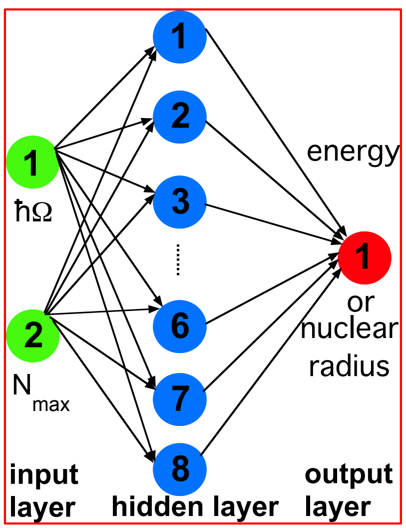
Deep Learning for Nuclear Binding Energy and Radius

Scientific Achievement

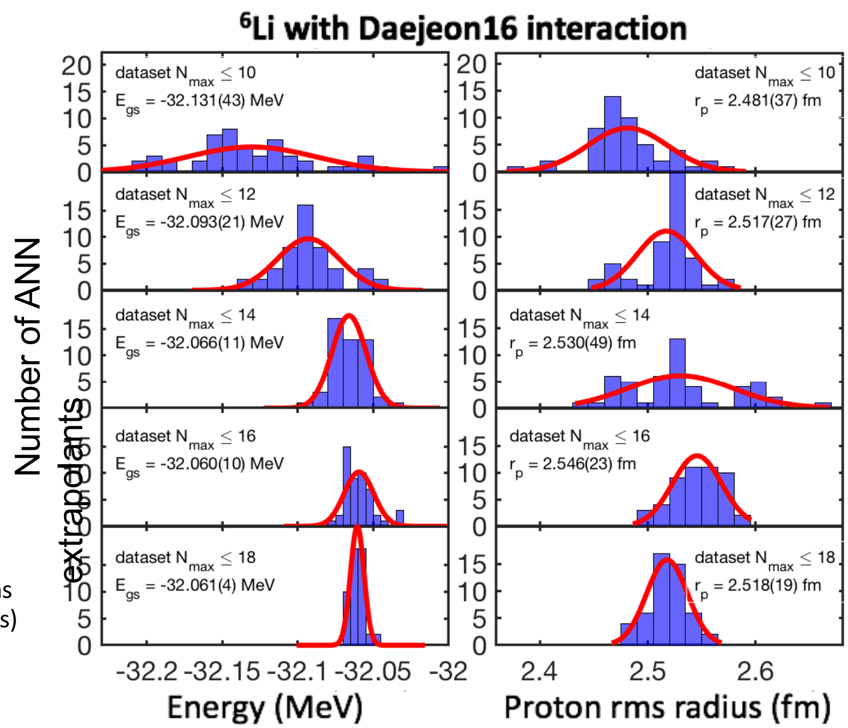
- Developed artificial neural networks (ANNs) for extending the application range of the *ab initio* No-Core Shell Model (NCSM)
- Demonstrated predictive power of ANNs for converged solutions of weakly converging simulations of the nuclear radius
- Provided a new paradigm for matching deep learning with results from high performance computing simulations

Significance and Impact

- Guides experimental programs at DOE's rare isotope facilities
- Extends the predictive power of *ab initio* nuclear theory beyond the reach of current high performance computing simulations
- Establishes foundation for deep learning tools in nuclear theory useful for a wide range of applications



Neural network **(above)** used to successfully extrapolate the ^{6}**Li** ground state energy and rms radius from modest basis spaces (N_{max} datasets) to extreme basis spaces achieving basis parameter independence (histograms of extrapolation ensembles in **right figure**).

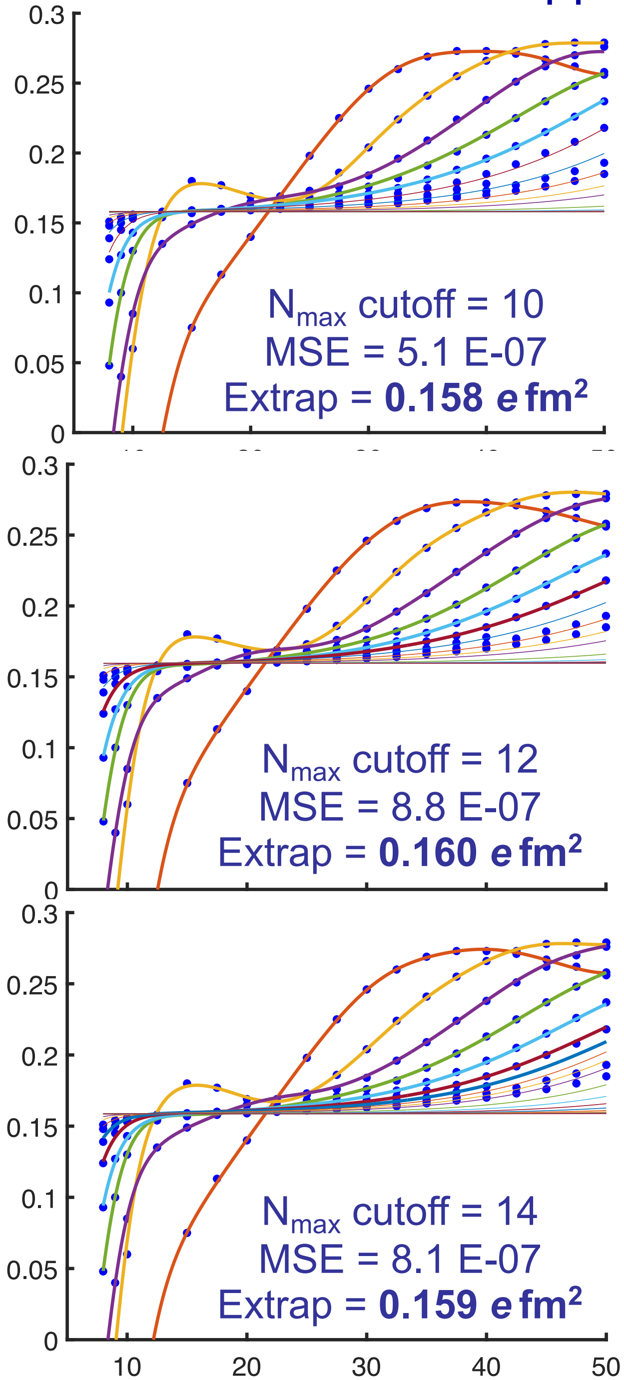


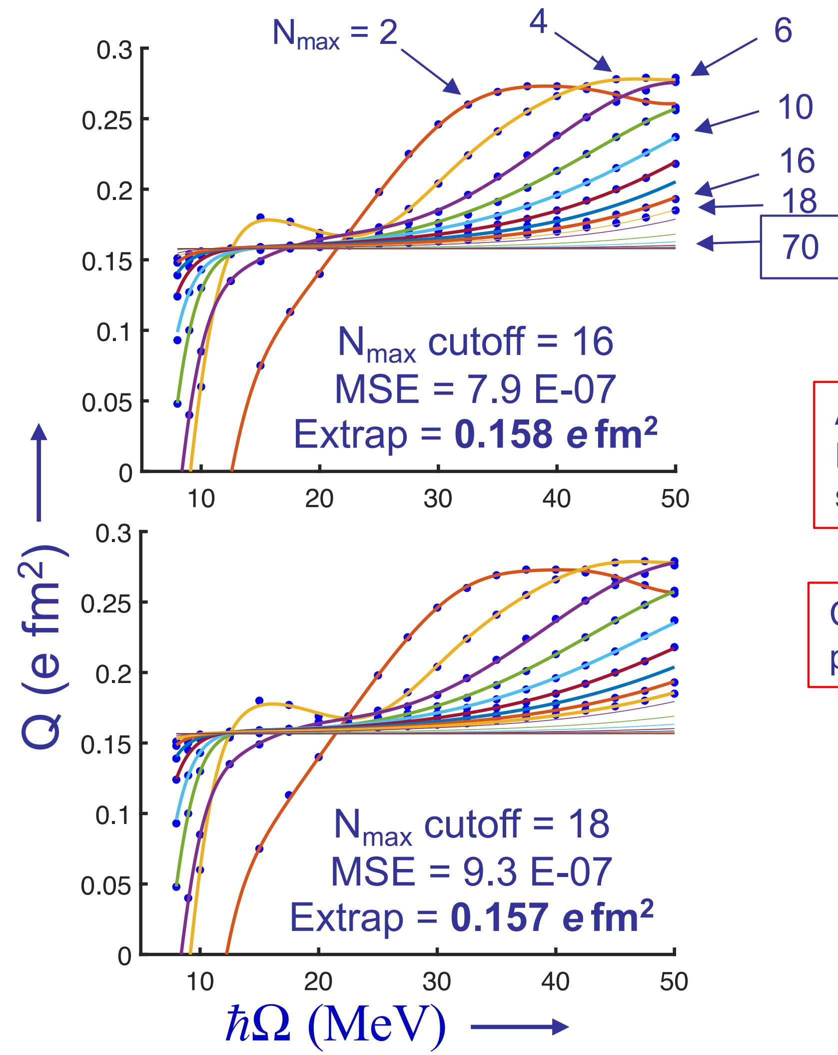
Research Details

- Develop ANNs that extend the reach of high performance computing simulations of nuclei
- Predict properties of nuclei based on *ab initio* structure calculations in achievable basis spaces
- Produce accurate predictions of nuclear properties with quantified uncertainties using fundamental inter-nucleon interactions such as Daejeon16

Ref: G. A. Negoita, et al., Phys. Rev. C **99**, 054308 (2019); https://journals.aps.org/prc/pdf/10.1103/PhysRevC.99.054308

Initial application to the ^{6}Li ground state quadrupole moment
“Best in Class”

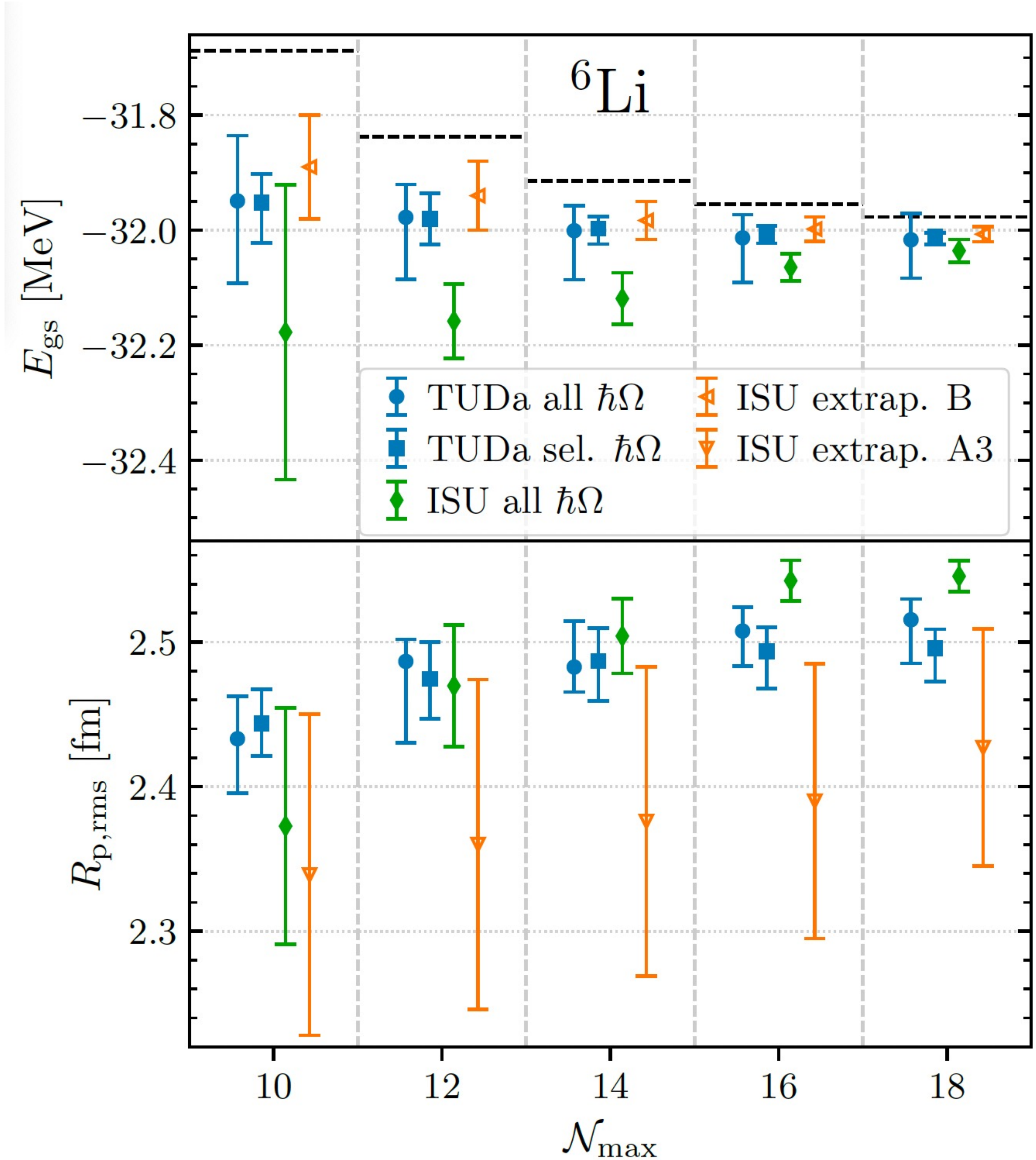




ANN predictions for N_{max} = 20, 25, . . . 65, 70 shown in all graphs

Converged sequence of ANN predictions: Q = 0.157(2) *e* fm^2

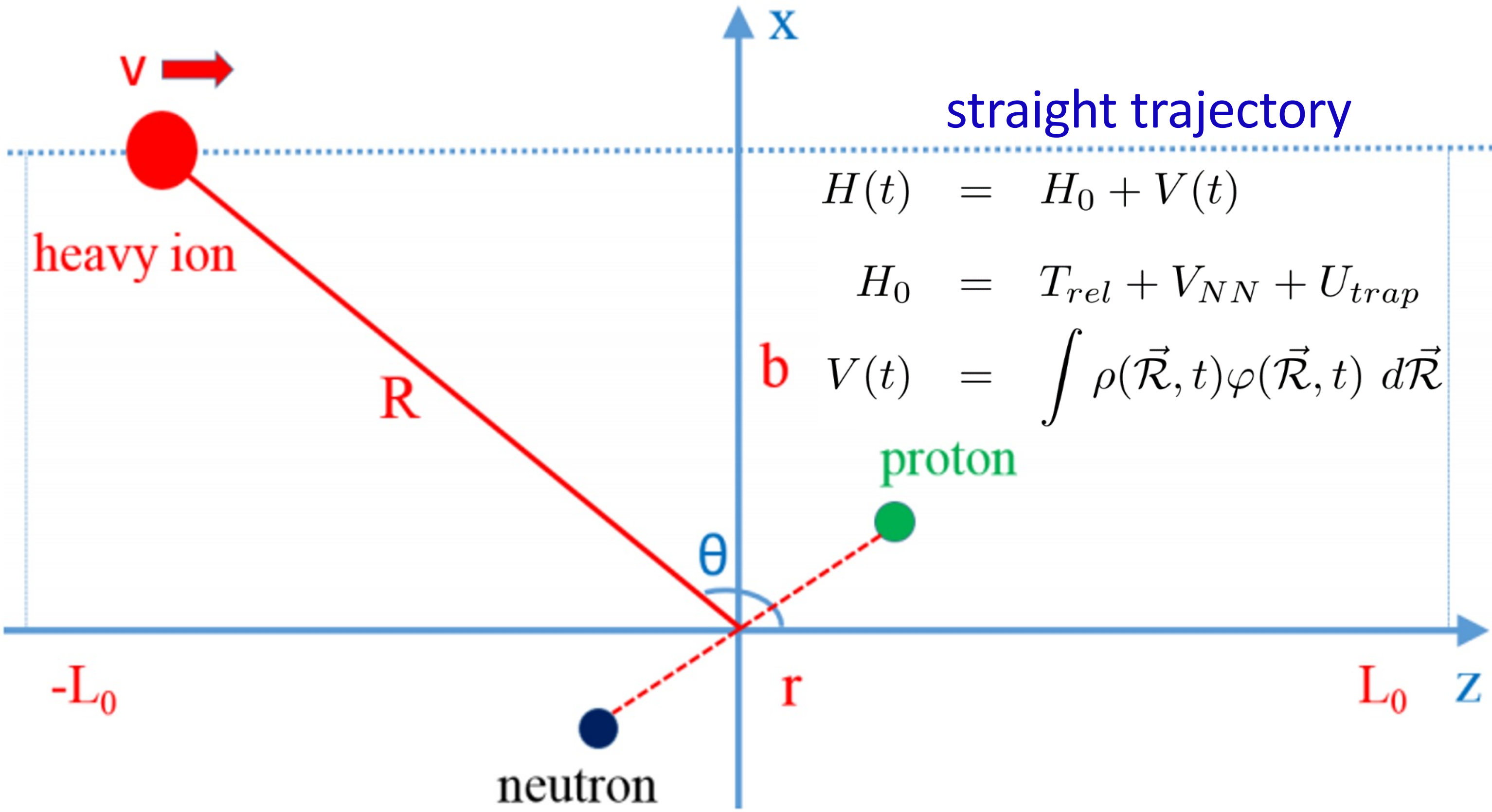
M. Lockner, R. McCarty, et al., in preparation



"Benchmarking ANN extrapolations of the ground state energies and rms radii of the Li isotopes,"
M. Knoll, M. Lockner, P. Maris, R.J. McCarty, R. Roth, J.P. Vary and T. Wolfgruber, in preparation

"TUD" – Technische Universitaet Darmstadt
"ISU" – Iowa State University

tBF on Quantum Computers
Demonstration case: Coulomb excitation of deuterium by peripheral scattering on a heavy ion

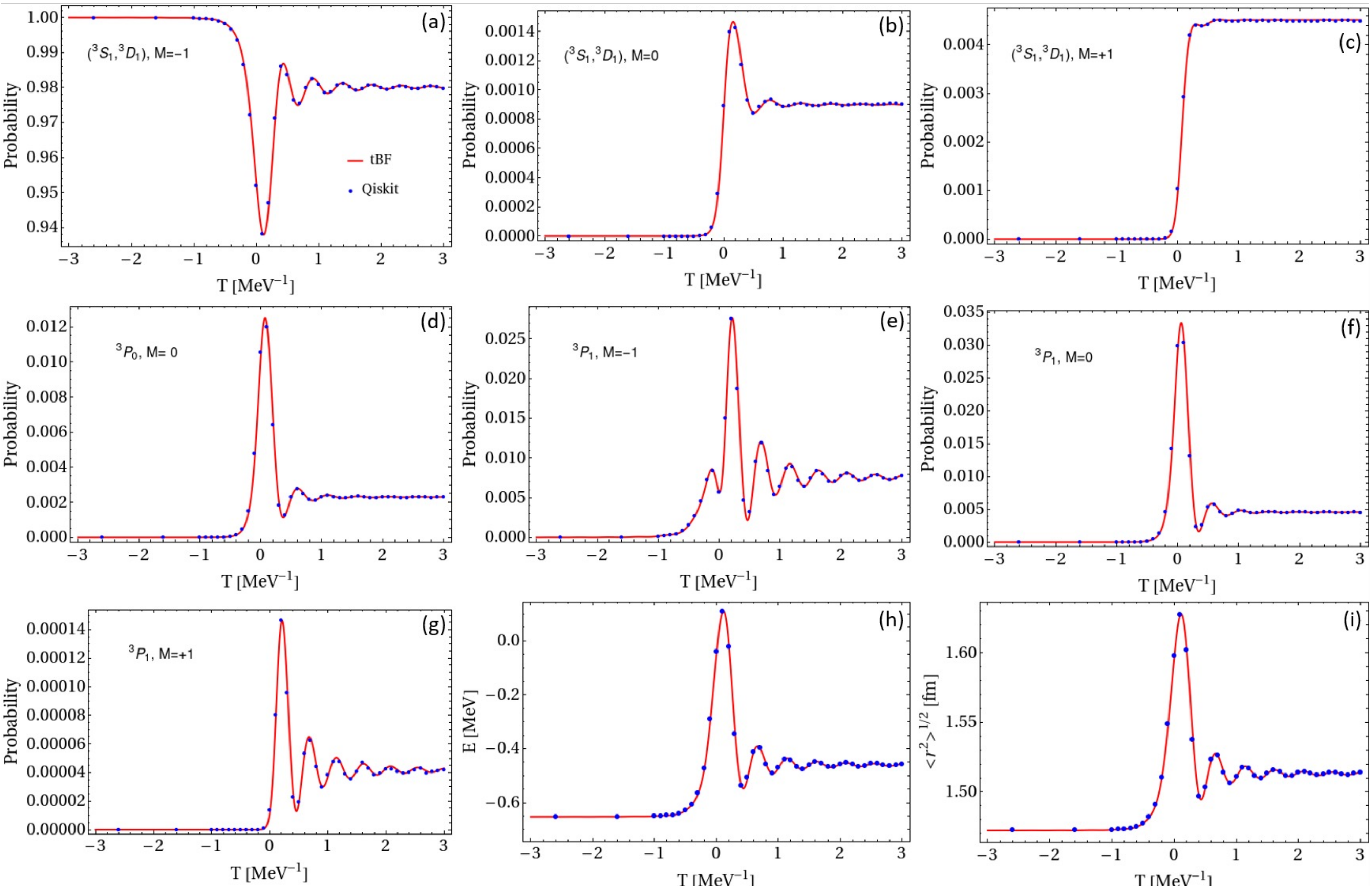


$$
\begin{aligned}
H(t) &= H_0 + V(t) \\
H_0 &= T_{rel} + V_{NN} + U_{trap} \\
V(t) &= \int \rho(\vec{\mathcal{R}}, t)\varphi(\vec{\mathcal{R}}, t)\, d\vec{\mathcal{R}}
\end{aligned}
$$

- H_0: Target (deuteron in trap) Hamiltonian
- φ: Coulomb field from heavy ion (U^{92+}) sensed by target
- ρ: Charge density distribution of target
- Limited to 7 deuteron states

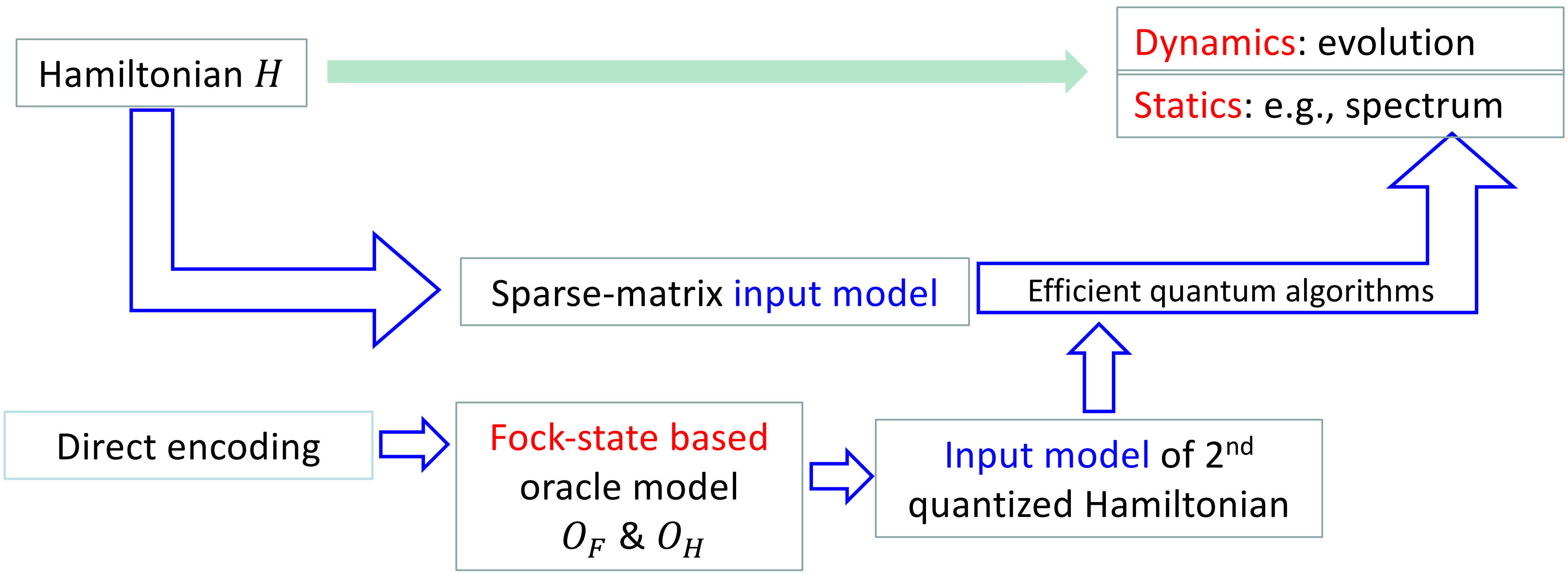
Previously solved with tBF: Weijie Du *et al.*, Phys. Rev. C 97, 064620 (2018)

Transition probabilities and observables



Weijie Du, James P. Vary, Xingbo Zhao and Wei Zuo, , Phys. Rev. A 104, 012611 (2021)

Quantum computing offers a promising path



Stage I:

W. Du and J.P. Vary, Phys. Rev. A 108, 052614 (2023)

Algorithmic design

Complexity analysis

Stage II

W. Du and J.P. Vary, arXiv: 2402.08969

Applications in many-fermion systems

Stage III

W. Du and J.P. Vary, arXiv: 2407.13672

Applications in many-boson systems

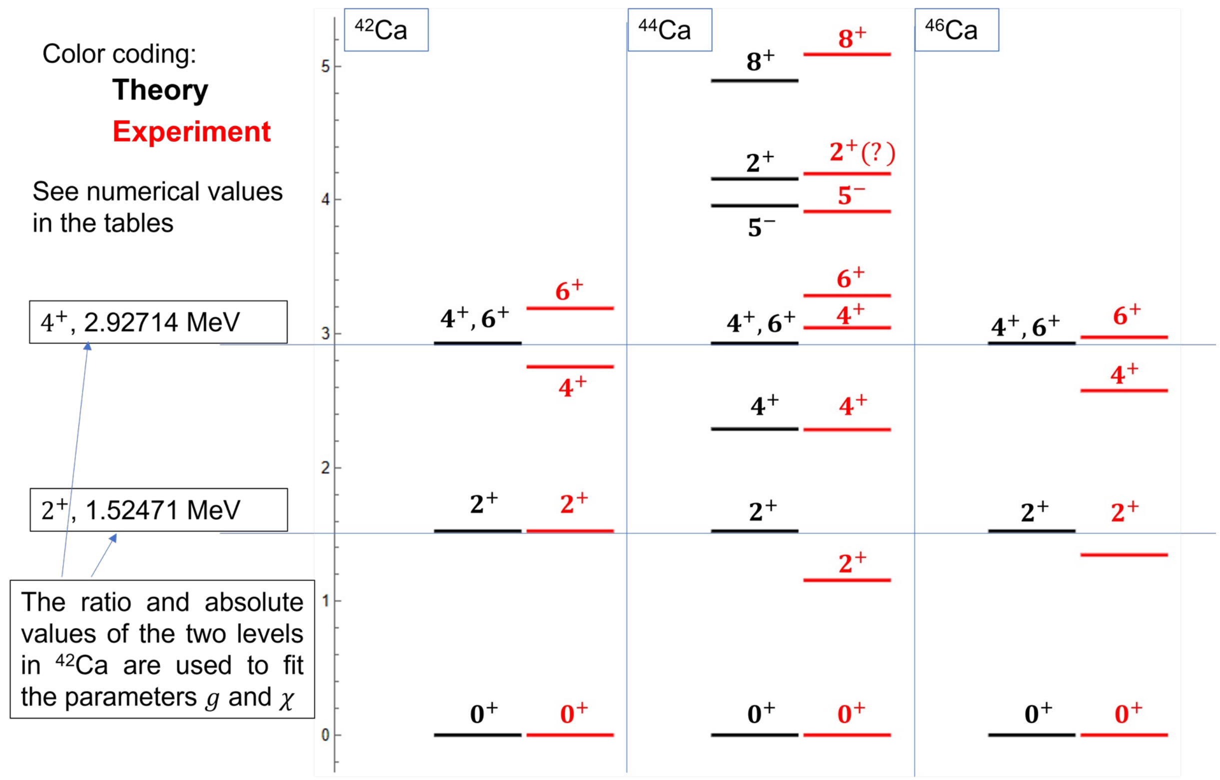
Application: Spectral calculations of ^{42}Ca, ^{44}Ca, and ^{46}Ca

- Pairing-plus-quadrupole-quadrupole interaction

$$H_A = g\left[-\sum_{\alpha,\beta} s_\alpha s_\beta a^\dagger_\alpha a^\dagger_{\bar{\alpha}} a_{\bar{\beta}} a_\beta + \chi \sum_{\alpha<\beta}\sum_{\gamma<\delta}\sum_{\mu=-2}^{2} \langle\alpha|r^2 Y_{2\mu}(\Omega_{\hat{r}})|\gamma\rangle\langle\beta|r^2 Y^*_{2\mu}(\Omega_{\hat{r}})|\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma\right]$$

- Basis space

	SP basis (qubit)	n	l	$2j$	$2m_j$	2τ
$0f_{7/2}$	**0**	0	3	7	$+7$	-1
	1	0	3	7	-7	-1
	2	0	3	7	$+5$	-1
	3	0	3	7	-5	-1
	4	0	3	7	$+3$	-1
	5	0	3	7	-3	-1
	6	0	3	7	$+1$	-1
	7	0	3	7	-1	-1



[W. Du and J.P. Vary, arXiv: 2402.08969]

[W. Du and J. P. Vary, in preparation]

Many outstanding nuclear physics puzzles and discoveries remain

Spin structure of the proton

Exotic systems including glueballs

Origin of successful constituent quark model

Origin of the successful nuclear shell model

Clustering phenomena

Nuclear reactions and breakup

Astrophysical processes & drip lines

Precision Nuclear Theory as a window on Physics beyond the Standard Model

Thank you for your attention

I welcome your questions