Nuclear Structure
Across Decades of Resolution

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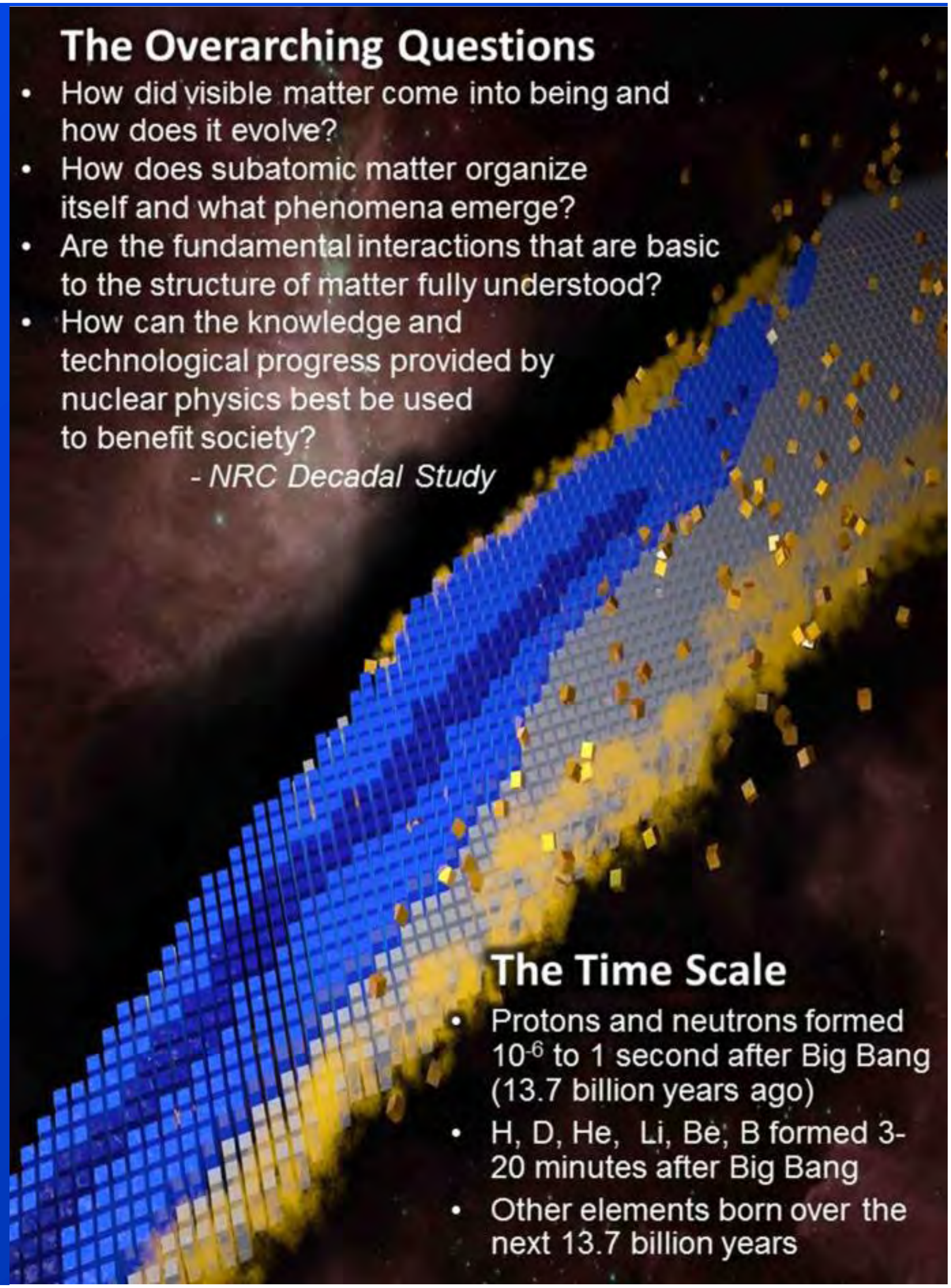
Nuclear Theory
in the
Supercomputer Era
(NTSE-2023)

IMP-CAS
Lanzhou

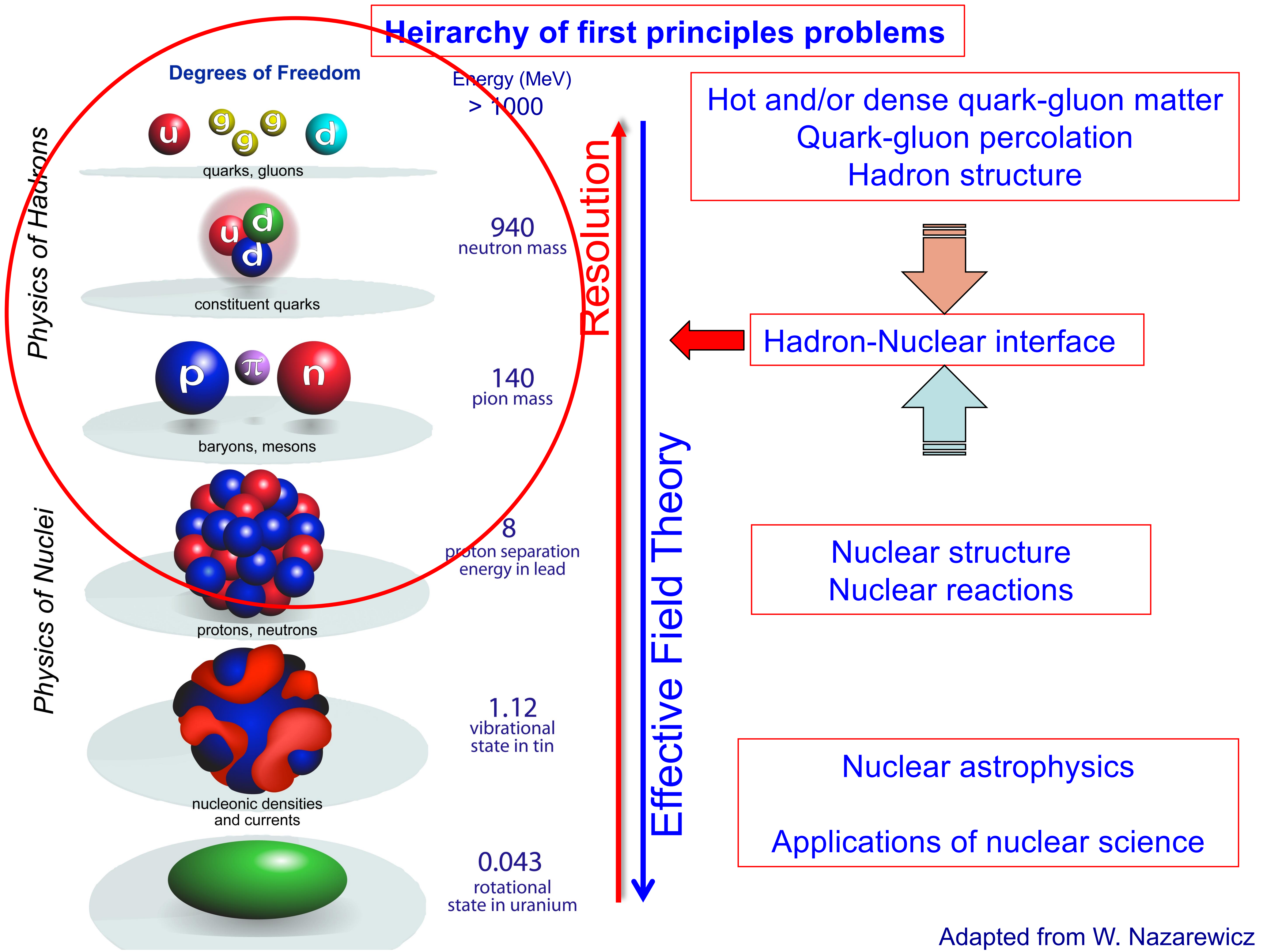
June 5, 2023



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?



Heirarchy of first principles problems
Degrees of Freedom
Energy (MeV)
> 1000
u
g
g
g
d
quarks, gluons
940
neutron mass
u
d
d
constituent quarks
140
pion mass
p
π
n
baryons, mesons
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

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.

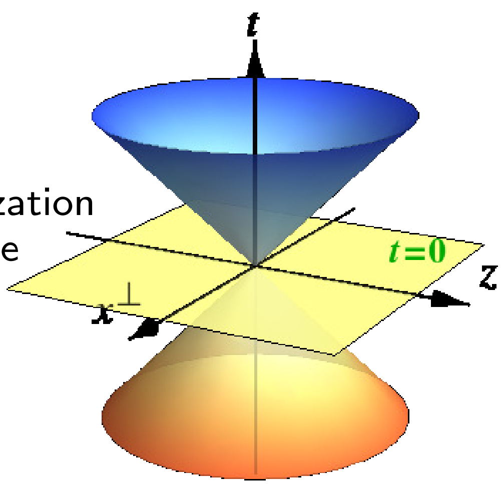
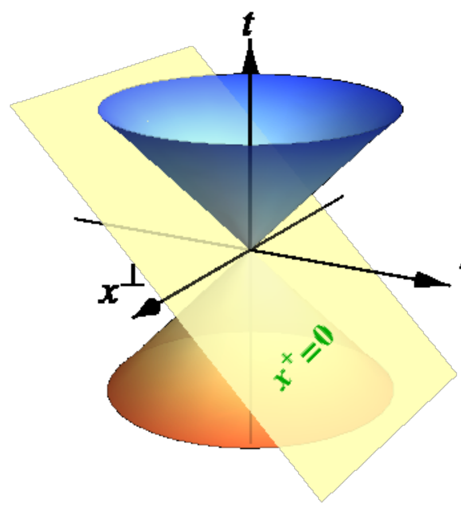
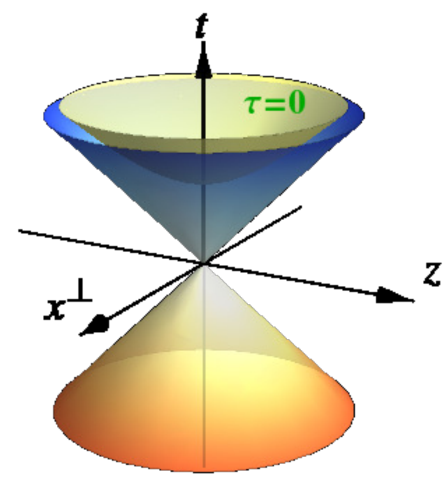
For the low-lying spectroscopy and reactions of the mesons and baryons, this could be an EFT of interacting constituent quarks and gluons.
Example: Basis Light Front Quantization (BLFQ) with Effective Hamiltonians inspired by Light-Front Holography with residual interactions from QCD.

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)

Let us first review the Basis Light Front Quantization (BLFQ) approach to the properties of the mesons and baryons and to their interactions

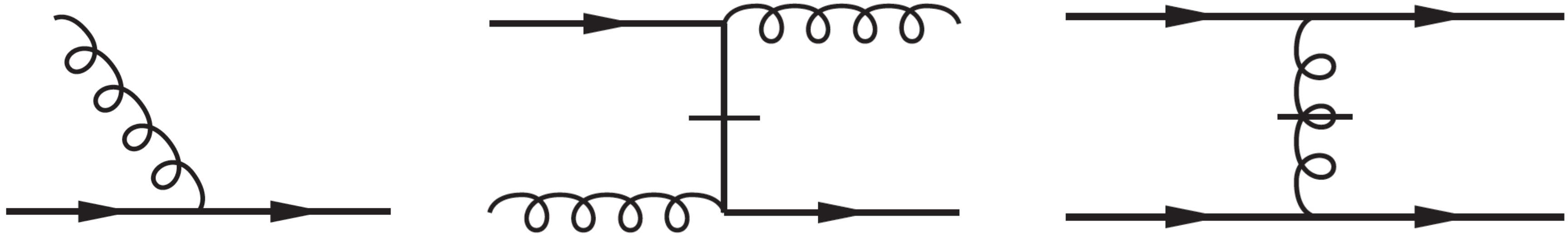
Dirac's forms of relativistic dynamics [Dirac, Rev. Mod. Phys. **21**, 392 1949]
Instant form is the well-known form of dynamics starting with $x^0 = t = 0$
$K^i = M^{0i}$, $J^i = \frac{1}{2}\varepsilon^{ijk} M^{jk}$, $\varepsilon^{ijk} = (+1,-1,0)$ for (cyclic, anti-cyclic, repeated) indeces
Front form defines relativistic dynamics on the light front (LF): $x^+ = x^0+x^3 = t+z = 0$

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

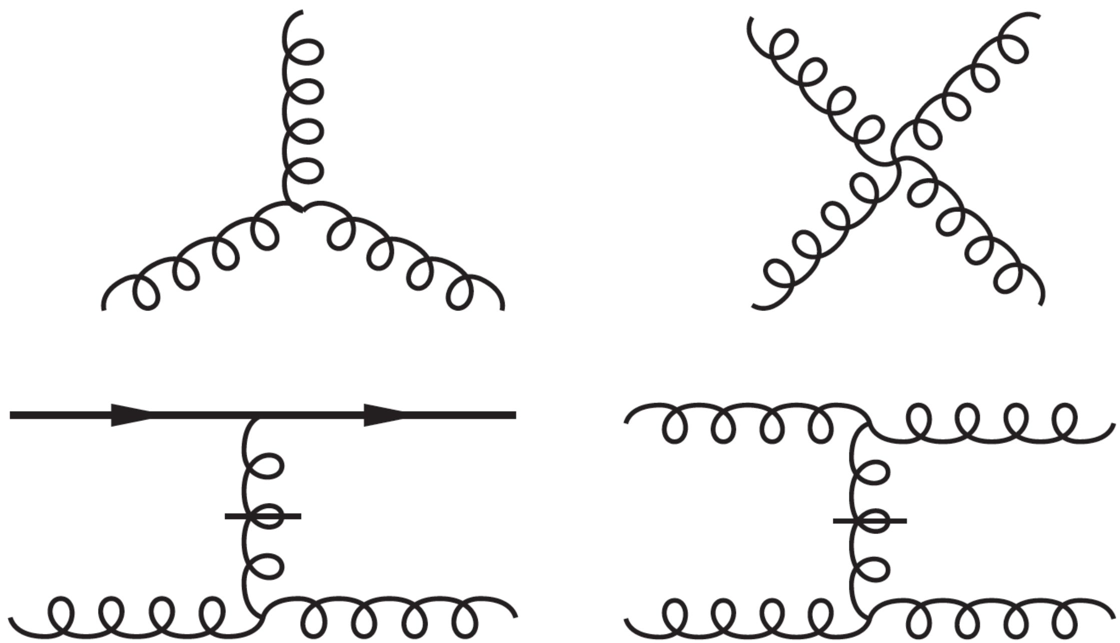
	instant form	front form	point form
time variable	$t = x^0$	$x^+ \triangleq x^0 + x^3$	$\tau \triangleq \sqrt{t^2 - \vec{x}^2 - a^2}$
quantization surface			
Hamiltonian	$H = P^0$	$P^- \triangleq P^0 - P^3$	P^μ
kinematical	$\vec{P}, \vec{J}$	$\vec{P}^\perp, P^+, \vec{E}^\perp, E^+, J^-$	$\vec{J}, \vec{K}$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

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, 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, $f_\alpha(\vec{x})$ 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)]

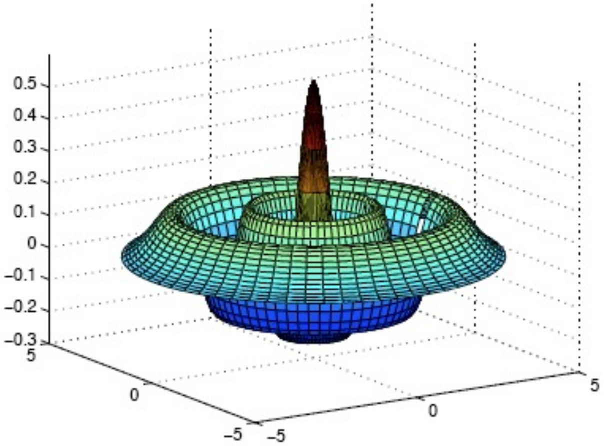
$$f_{\alpha=\{nml\}}\left(\vec{k}_\perp, x\right) = \phi_{nm}\left(\vec{k}_\perp / \sqrt{x(1-x)}\right)\chi_l(x)$$

ϕ_{nm} 2D-HO functions as in AdS/QCD

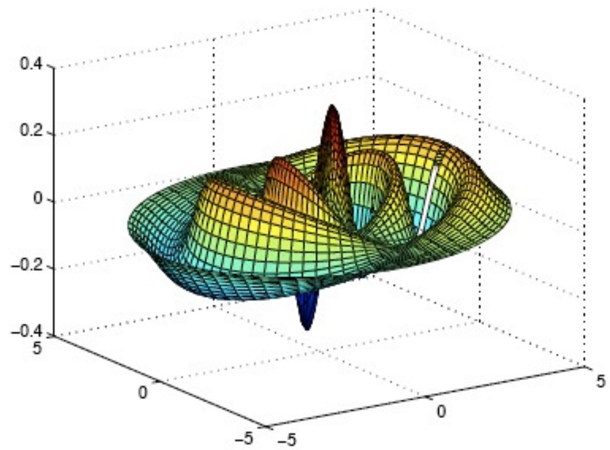
χ_l Jacobi polynomials times $x^a(1-x)^b$

Set of Transverse 2D HO Modes for n=4

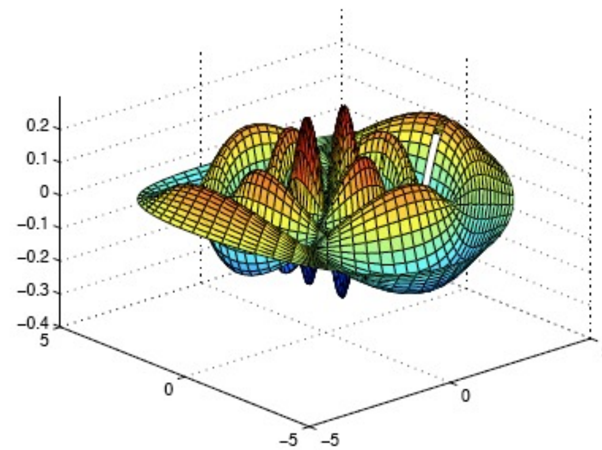
m=0



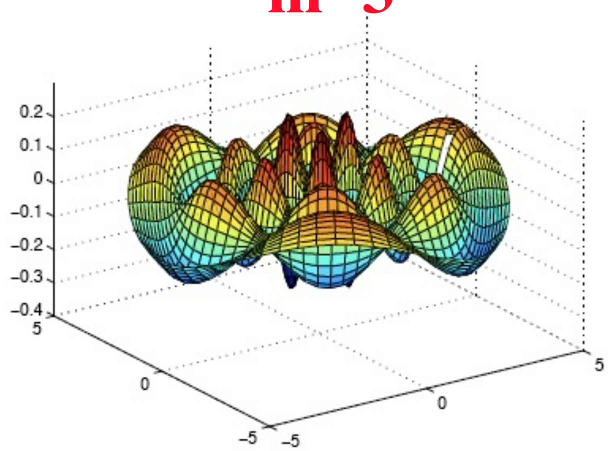
m=1



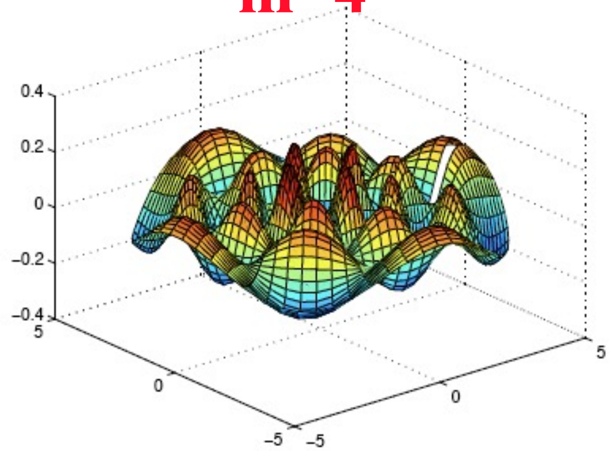
m=2



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

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

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

Global Color Singlets (QCD)

Light Front Gauge

Optional Fock-Space Truncation

All $J \geq J_z$ states in one calculation

Finite basis regulators

Preserve transverse boost invariance

Light-Front Wavefunctions (LFWFs)

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

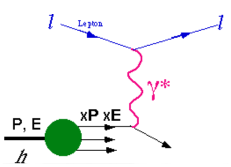
LFWFs are *frame-independent* (boost invariant) and depend only on the relative variables: $x_i \equiv p_i^+/P^+, \vec{k}_{i\perp} \equiv \vec{p}_{i\perp} - x_i \vec{P}_\perp$

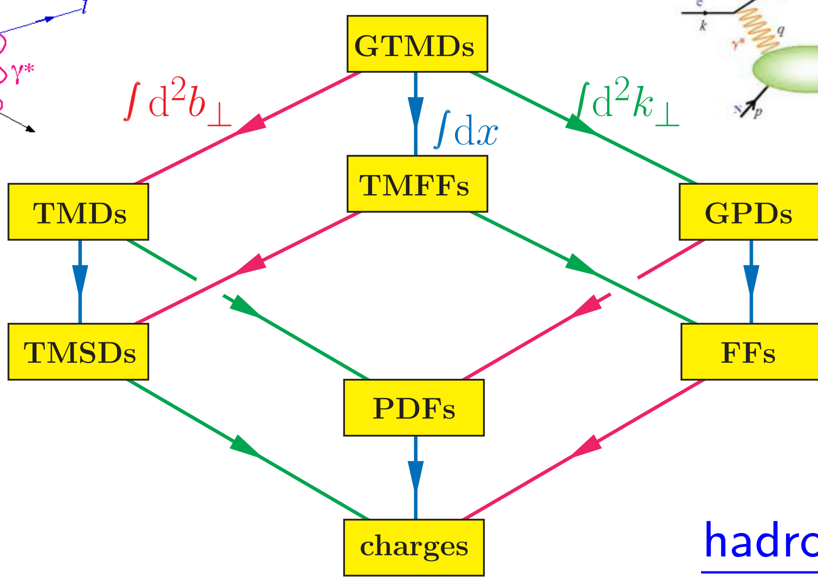
LFWFs provide intrinsic information of the structure of hadrons, and are indispensable for exclusive processes in DIS [Lepage '80]

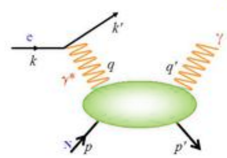
- Overlap of LFWFs: structure functions (e.g. PDFs), form factors, ...
- Integrating out LFWFs: light-cone distributions (e.g. DAs)

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

— Stanley J. Brodsky

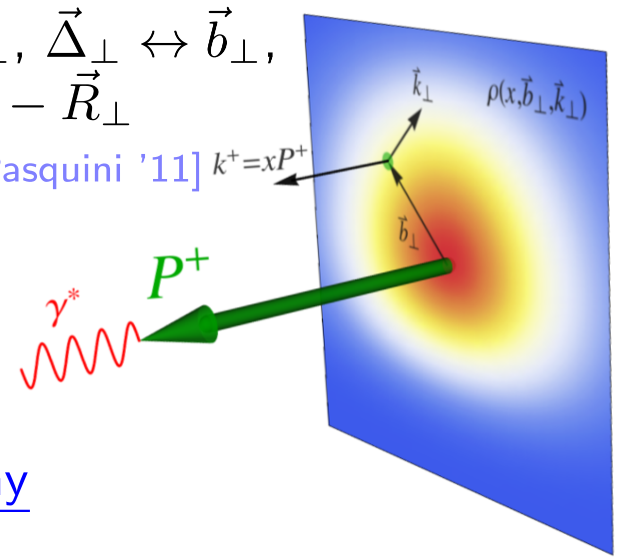






$\vec{k}_\perp \leftrightarrow \vec{r}_\perp$, $\vec{\Delta}_\perp \leftrightarrow \vec{b}_\perp$,
$\vec{b}_\perp = \vec{r}_\perp - \vec{R}_\perp$

[Lorcé & Pasquini '11]



hadron tomography

Overview of BLFQ/tBLFQ applications to mesons and baryons

Common features

Transverse confinement from 2D HO (in common with LF Holography)
Longitudinal confinement (Y. Li, et al, PLB 2016, PRD 2017)
Basis states from exact solutions of a reference Hamiltonian
Compare results with experiment, lattice, DSE/BSE, . . .

Distinct features

For Veff
1) perturbative one-gluon exchange (Y. Li, et al, PLB 2016, PRD 2017)
2) NJL model for light meson applications (S. Jia, et al, PRC 2019)

For Fock space truncation
1) Valence sector
2) Valence sector plus dynamical gluon (plus sea quarks, plus …)

For observables
1) Single state properties and decays
2) Transitions between states
3) Non-perturbative probes (tBLFQ)

Next Methods

BLFQ on Quantum Computers

Heavy Quarkonia

[Y. Li, et al., Phys. Letts. B 758, 118 (2016); Phys. Rev. D 96, 016022 (2017)]

- The effective Hamiltonian:

$$H_{\text{eff}} = \overbrace{\underbrace{\frac{\vec{k}_\perp^2 + m_q^2}{x} + \frac{\vec{k}_\perp^2 + m_{\bar{q}}^2}{1-x}}_{\text{LF kinetic energy}} + \underbrace{\kappa^4 x(1-x)\vec{r}_\perp^2 - \frac{\kappa^4}{(m_q+m_{\bar{q}})^2}\frac{\partial}{\partial x}\Big(x(1-x)\frac{\partial}{\partial x}\Big)}_{\text{confinement}}}^{H_0} + \underbrace{V_g}_{\text{one-gluon exchange}}$$

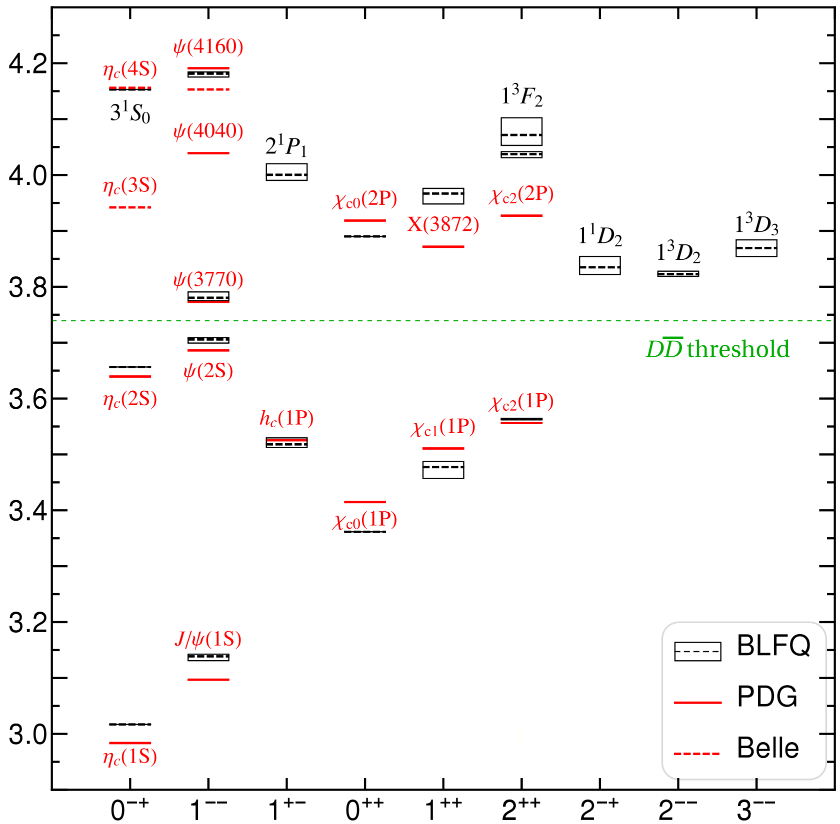
where $x = p_q^+/P^+$, $\vec{k}_\perp = \vec{p}_{q\perp} - x\vec{P}_\perp$, $\vec{r}_\perp = \vec{r}_{q\perp} - \vec{r}_{\bar{q}\perp}$.

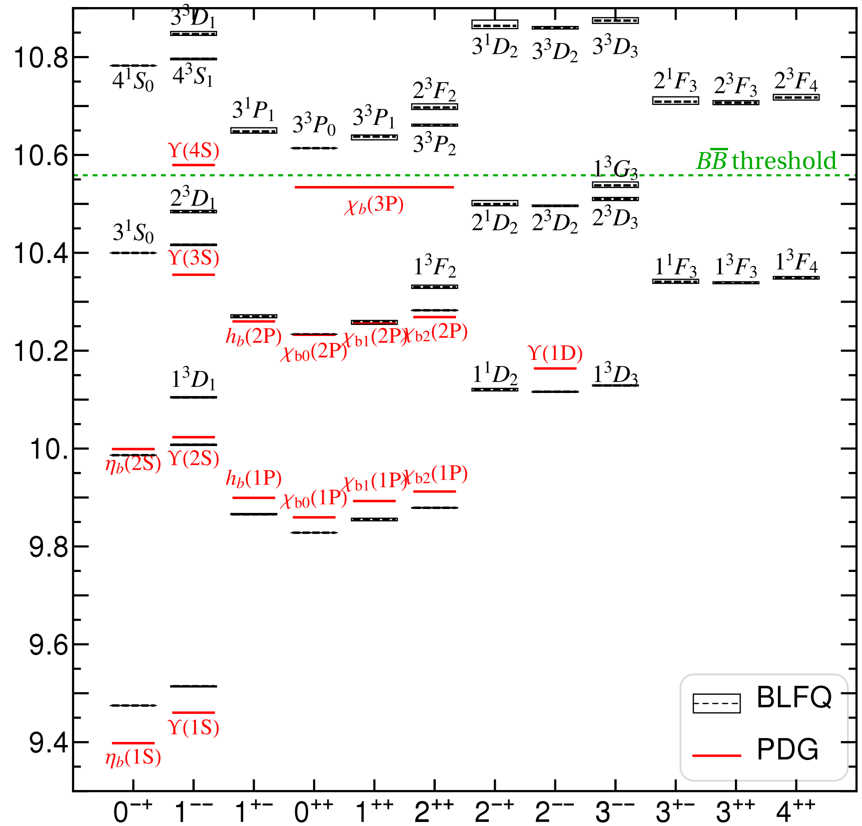
  - Confinement
    transverse holographic confinement [S.J.Brodsky,PR584,2015]
    longitudinal confinement [Y.Li,PLB758,2016]
  - One-gluon exchange with running coupling
    $V_g = -\frac{4}{3}\frac{4\pi\alpha_s(Q^2)}{Q^2}\bar{u}_{\sigma'}\gamma^\mu u_\sigma \bar{v}_s \gamma_\mu v_{s'}$ [M.Krautgartner:PRD45,1992]

- Basis representation
  - valence Fock sector: $|q\bar{q}\rangle$ (initially)
  - basis functions: eigenfunctions of H_0 (LF kinetic energy+ confinement)

Spectroscopy

[Y. Li, et al., Phys. Letts. B 758, 118 (2016); Phys. Rev. D 96, 016022 (2017)]





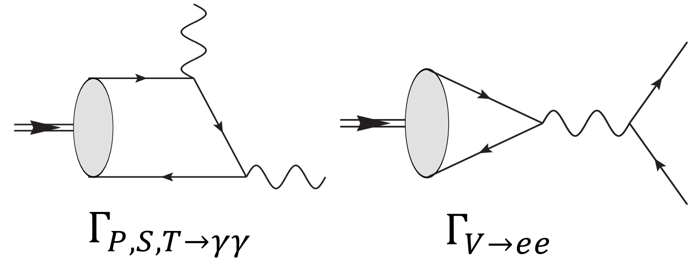
	κ (GeV)	m_q (GeV)	rms (MeV)	$\overline{\delta_J M}$ (MeV)	$N_{\max}$	basis dim.
$c\bar{c}$	0.966	1.603	31	17	32	1812
$b\bar{b}$	1.389	4.902	38	8	32	1812

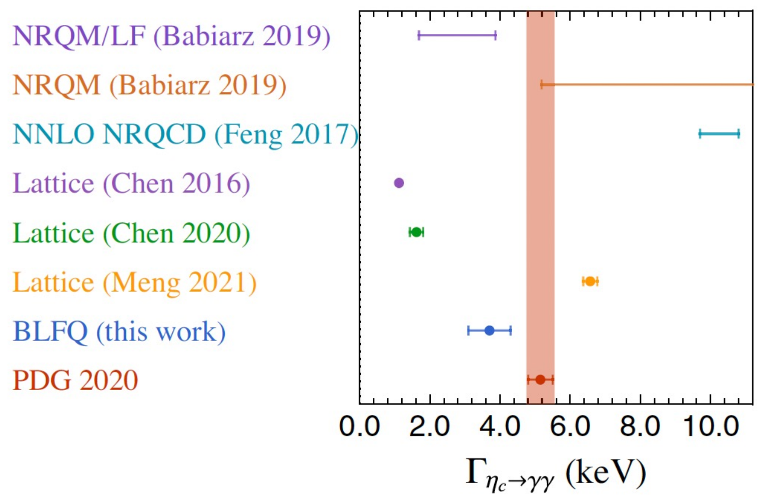
κ determined from fits to spectrum follows the HQET trajectory $\kappa_h \propto \sqrt{M_h}$, in agreement with recent LFH result [Dosch et al, PRD**95** (2017)]

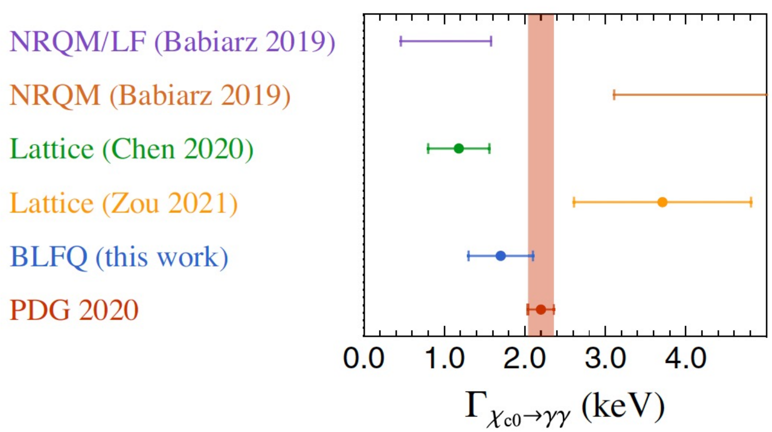
Yang Li, Meijian Li and James P. Vary, PRD 105, L071901 (2022)

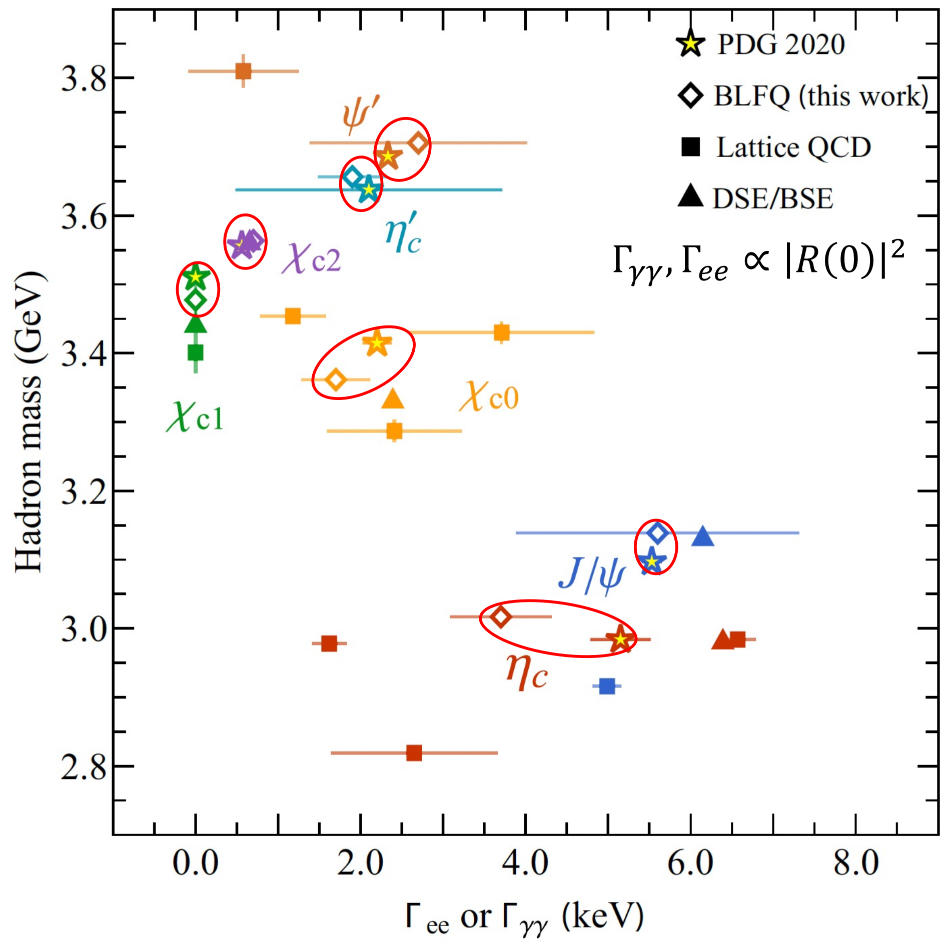
Diphoton width $\Gamma_{\gamma\gamma}$ of charmonia in BLFQ

- ✓ Notoriously challenging
- ✓ BLFQ predictions are very competetive!
  - ✓ No parameters were adjusted!





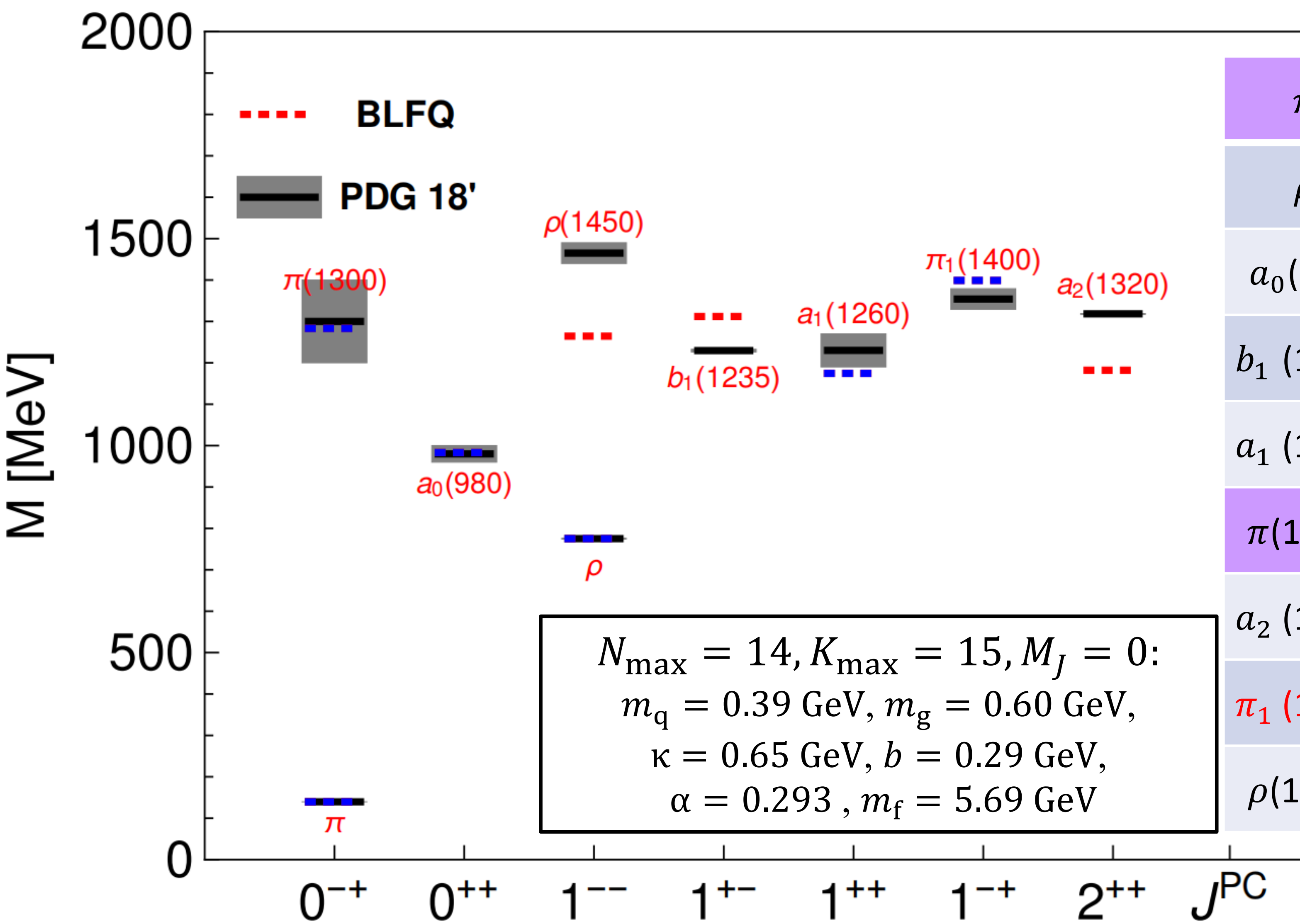




Lattice: Dudek '06, Chen '16, Chen '20, Meng '21, Zou '21;
NRQCD: Feng '15 & '17
NRQM: Babiarz '19 & '20

Comparison of theoretical prediction of masses and dilepton/diphoton widths combined

Light Meson Mass Spectrum Including One Dynamical Gluon



	Norm$q\bar{q}$	DC[MeV]
π	0.492	138
ρ	0.486	129
$a_0(980)$	0.370	0
b_1 (1235)	0.30	0
a_1 (1260)	0.324	11
$\pi(1300)$	0.284	53
a_2 (1320)	0.320	0
π_1 (1400)	0.002	0
$\rho(1450)$	0.312	46

$N_{\max} = 14, K_{\max} = 15, M_J = 0:$
$m_q = 0.39$ GeV, $m_g = 0.60$ GeV,
$\kappa = 0.65$ GeV, $b = 0.29$ GeV,
$\alpha = 0.293$, $m_f = 5.69$ GeV

$$|\text{meson}\rangle = a|q\bar{q}\rangle + b|q\bar{q}g\rangle + \cdots$$

Fix the parameters by fitting six blue states

- $\pi_1(1400)$: $|q\bar{q}g\rangle$ dominates
- $\pi(1300)$: Decay Constant (DC) < π's DC

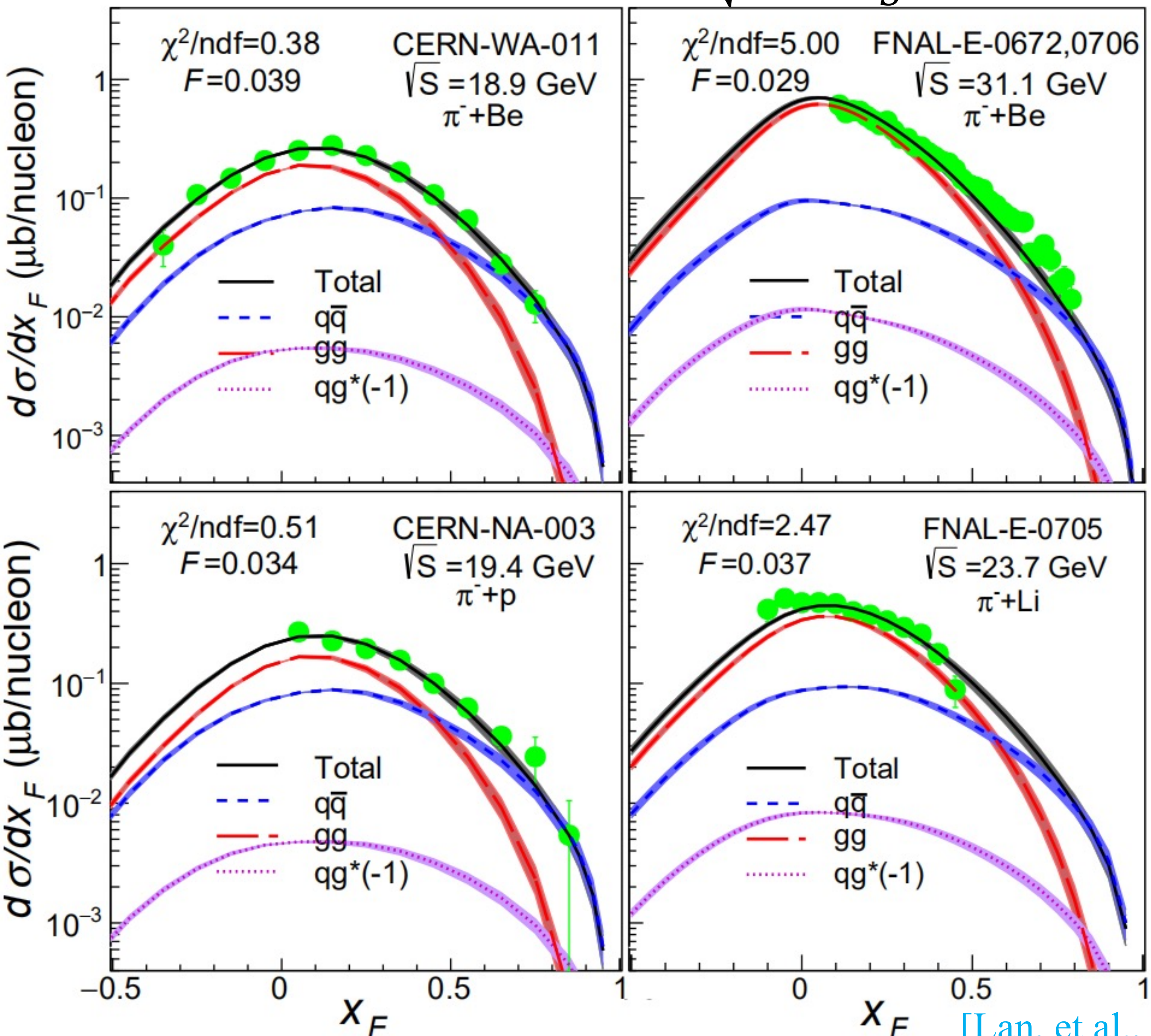
[Lan, et al., (BLFQ Collaboration) PLB 825, 136890 (2022); arXiv 2106.04954]

J/ψ production cross section

$\pi^{\pm} N \rightarrow J/\psi\ X$

$$\frac{d\sigma}{dx_F}[J/\psi] = F \sum_{i,j=q,\bar{q},g} \int_{2m_c}^{2m_D} dM_{c\bar{c}} \frac{2M_{c\bar{c}}}{S\sqrt{x_F^2 + \frac{4M_{c\bar{c}}^2}{S}}} \hat{\sigma}_{ij}(s, m_c^2, \mu_R^2, \mu_F^2) f_i^{\pi^{\pm}}(x_1, \mu_F^2) f_j^N(x_2, \mu_F^2)$$

[nCTEQ 2015]



CEM

[Chang, et al, PRD 102 (2020) 054024];
[Nason, et al, NPB 303 (1988) 607];
[Mangano, et al, NPB 405 (1993) 507]

Agree with experimental data (FNAL E672, E706, E705, CERN NA3,WA11).

[Lan, et al., PLB 825, 136890 (2022)]

BLFQ Basis States

- BLFQ basis: expansion in Fock space

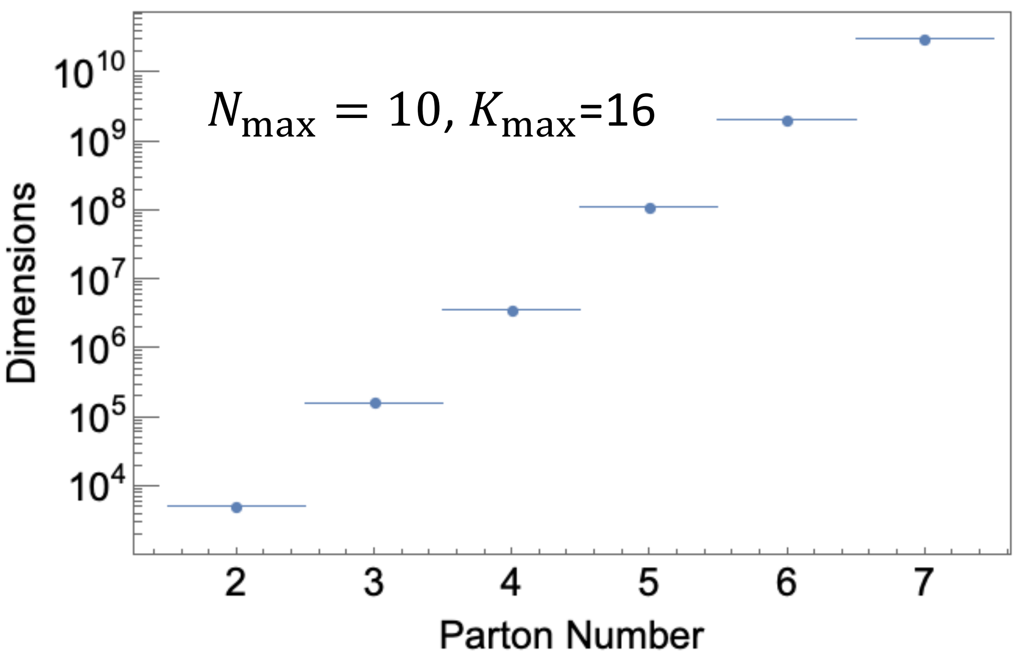
$$|\beta_{\rm meson}\rangle = |q\bar{q}\rangle + |q\bar{q}g\rangle + |gg\rangle + |q\bar{q}\ q\bar{q}\rangle + |q\bar{q}\ gg\rangle + |q\bar{q}\ q\bar{q}\ g\rangle + |q\bar{q}q\bar{q}gg\rangle + \cdots$$

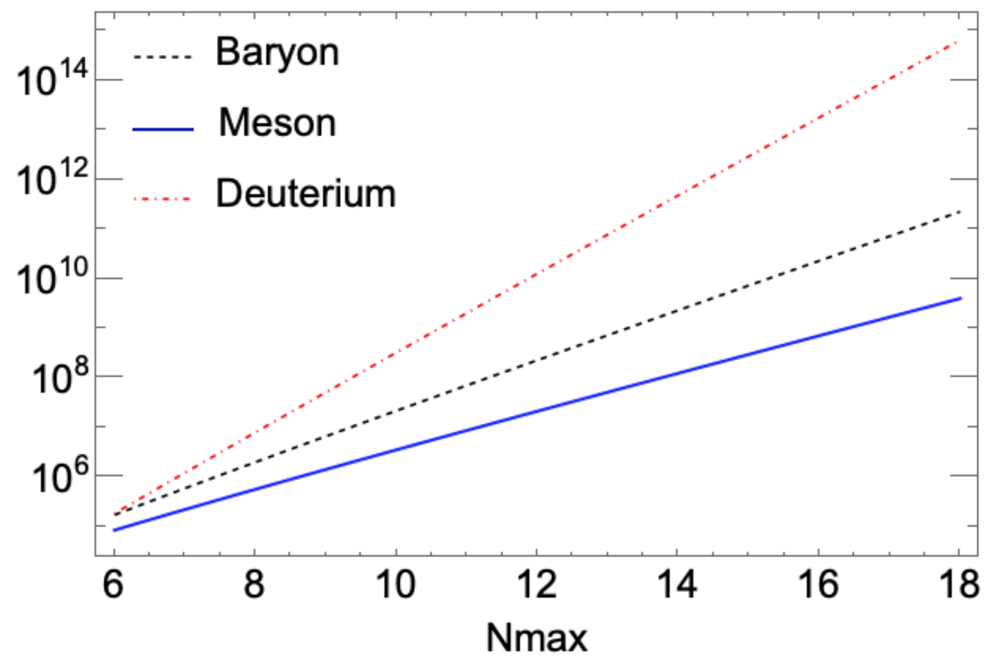
$$|\beta_{\rm baryon}\rangle = |qqq\rangle + |qqqg\rangle + |qqq\ q\bar{q}\rangle + |qqq\ gg\rangle + |qqq\ q\bar{q}g\rangle + |qqqq\bar{q}gg\rangle + \cdots$$

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

- Dimension of basis states increases with number of Fock sectors

=> motivation for quantum computing





Baryons with one dynamical gluon

$$|P_{baryon}\rangle = \Psi_1|qqq\rangle + \Psi_2|qqqg\rangle$$

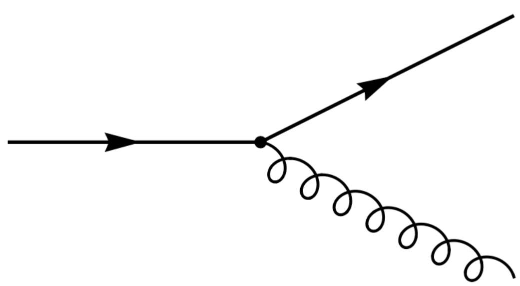
$$P^- = H_{K.E.} + H_{trans} + H_{longi} + H_{Interact}$$

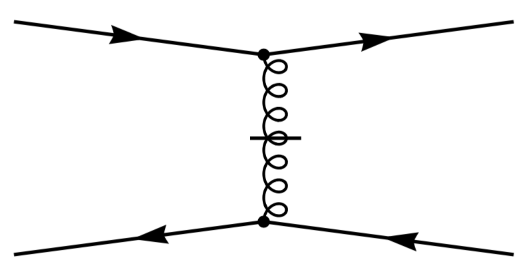
$$H_{K.E.} = \sum_i \frac{p_i^2 + m_q^2}{p_i^+}$$

$$H_{trans} \sim \kappa_T^4 r^2$$ -- Brodsky, Teramond arXiv: 1203.4025

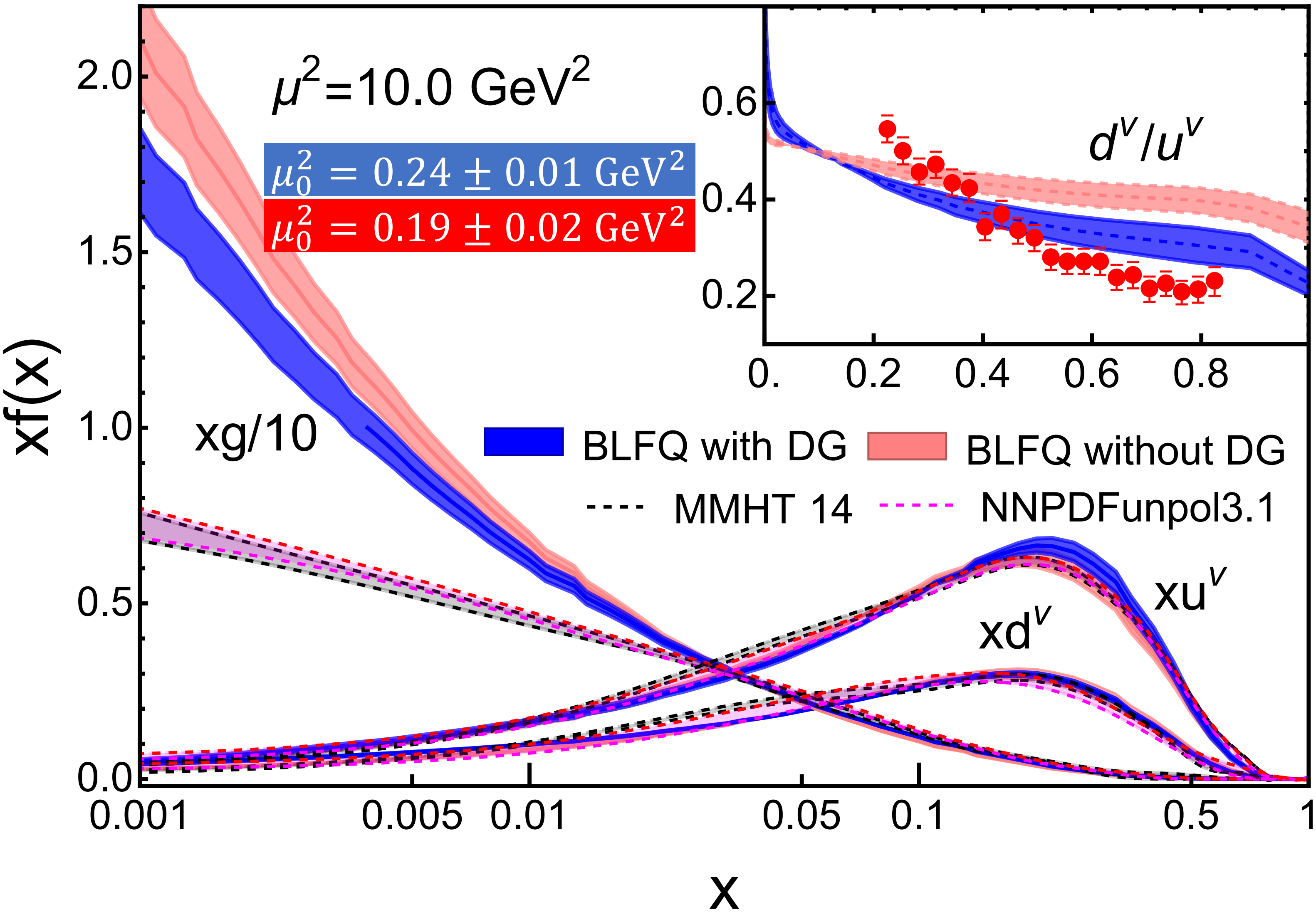
$$H_{longi} \sim -\sum_{ij} \kappa_L^4 \partial_{x_i}\left(x_i x_j \partial_{x_j}\right)$$ ---Y Li, X Zhao , P Maris , J Vary, PLB 758(2016)

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





Unpolarized Parton Distribution Functions



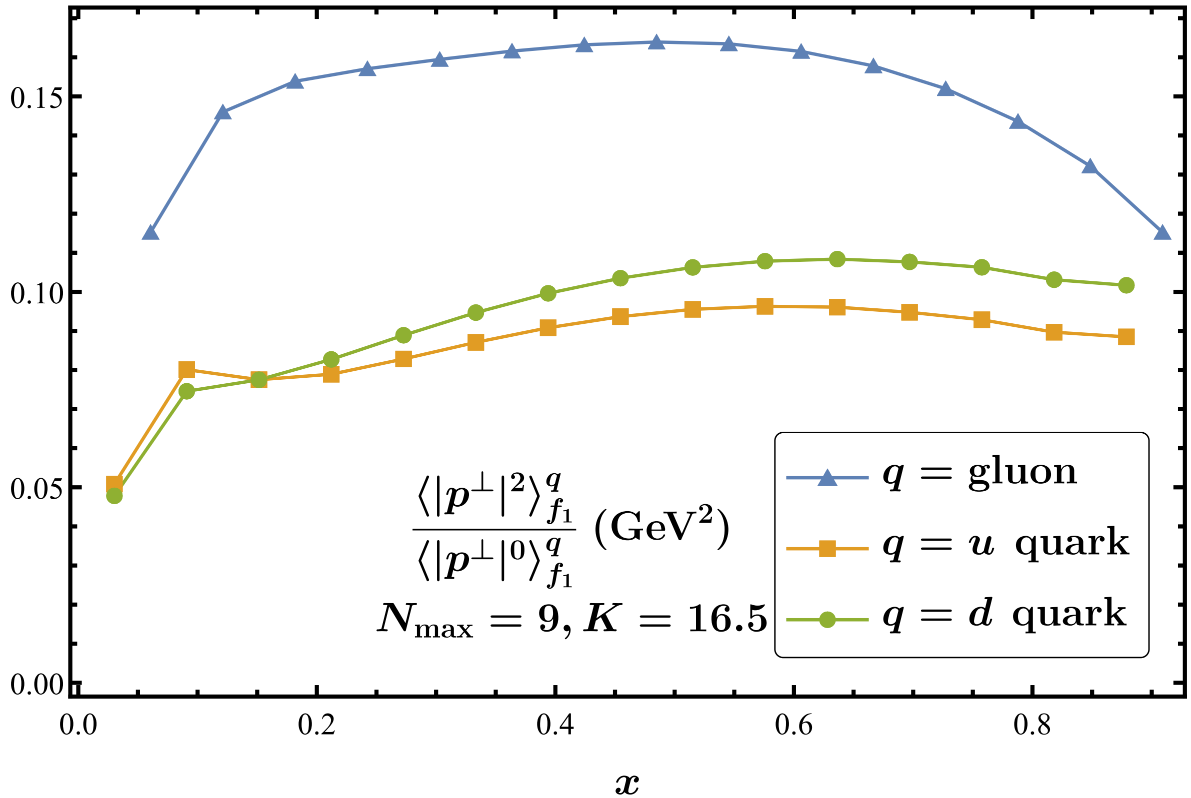
The data point are extracted from MARATHON data

Including the One Dynamical Gluon Fock Sector, the gluon distribution is closer to the global fit.

S. Xu, CM, X. Zhao, Y. Li, J. P. Vary, 2209.08584 [hep-ph].

[EPJC 77 (2017) 663]

Average transverse momentum of quark and gluon



- After integrating over x, we further obtain
  g: 0.156 (GeV)^2
  u: 0.082 (GeV)^2
  d: 0.083 (GeV)^2

- Define $\langle|p^\perp|^n\rangle^q_{f_1} = \int d^2p^\perp\, |p^\perp|^n \times f_1^q$ then we know that $\frac{\langle|p^\perp|^2\rangle^q_{f_1}}{\langle|p^\perp|^0\rangle^q_{f_1}}$ would be the average transverse momentum of flavor q
- Average transverse momentum of d quark is slightly larger than that of u, the same as our $|qqq\rangle$ Fock sector conclusion.
- With $|qqqg\rangle$ Fock sector we now also know that transverse momentum of gluon is larger than that of quark

Zhi Hu, et al., in preparation

Forward quark jet-nucleus scattering in light-front Hamiltonian approach

Time-dependent Basis Light-Front Quantization (tBLFQ)

❖ First-principles:

In the light-front Hamiltonian formalism, the state obeys the time-evolution equation, and the Hamiltonian is derived from the QCD Lagrangian

$$\frac{1}{2}P^-(x^+)|\psi(x^+)\rangle = i\frac{\partial}{\partial x^+}|\psi(x^+)\rangle$$

❖ Nonperturbative treatment:

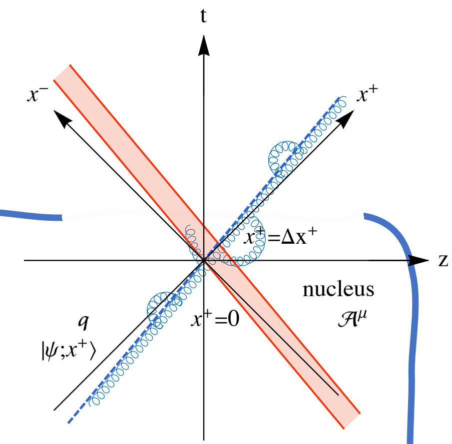
The time evolution operator is divided into many small timesteps, each timestep is evaluated numerically and intermediate states are accessible,

$$|\psi(x^+)\rangle = \mathcal{T}_+ \exp\left[-\frac{i}{2}\int_0^{x^+} dz^+ P^-(z^+)\right]|\psi(0)\rangle$$

$$= \lim_{n\to\infty}\prod_{k=1}^{n} \mathcal{T}_+ \exp\left[-\frac{i}{2}\int_{x_{k-1}^+}^{x_k^+} dz^+ P^-(z^+)\right]|\psi(0)\rangle$$

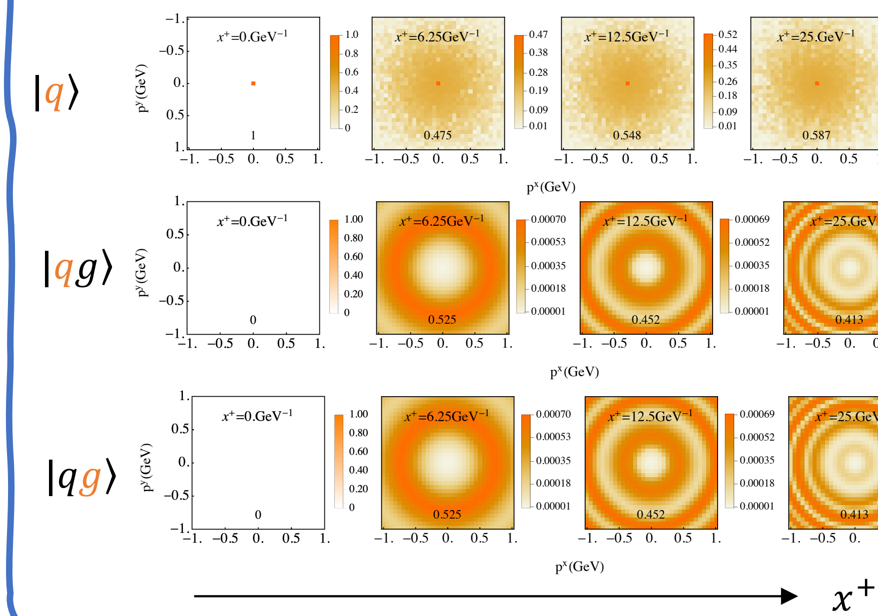
❖ Basis representation:

Optimal basis has the same symmetries of the system, and it is the key to numerical efficiency



We consider scattering of a high-energy quark moving in the positive z direction, on a high-energy nucleus moving in the negative z direction.

Time evolution of a quark state in the $|q\rangle + |qg\rangle$ Fock space observed from the transverse momentum space



M. Li, T. Lappi and X. Zhao, Phys. Rev. D 104, 056104 (2021)

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

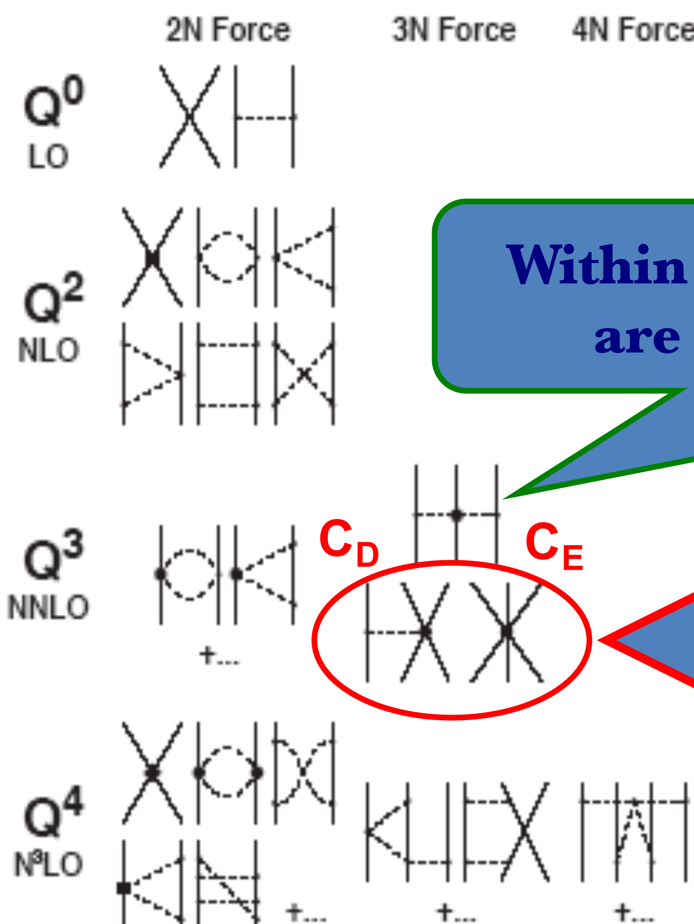
Effective Nucleon Interaction

(Chiral Perturbation Theory)

Chiral perturbation theory (χPT) allows for controlled power series expansion

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

$\Lambda_\chi \approx 1\ GeV$, χ - symmetry breaking scale



Within χPT 2π-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 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)

No Core Shell Model (NCSM)

A large sparse matrix eigenvalue problem

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

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

$$\left|\Psi_i\right\rangle = \sum_{n=0}^{\infty} A_n^i \left|\Phi_n\right\rangle$$

$$\text{Diagonalize } \left\{\left\langle\Phi_m\right|H\left|\Phi_n\right\rangle\right\}$$

- Adopt realistic NN (and NNN) interaction(s) & renormalize as needed - retain induced many-body interactions: Chiral Effective Field Theory (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 bookkeepping of anti-symmetrization)
- Diagonalize this sparse many-body H in its "m-scheme" basis where [α =(n,l,j,m_j,τ_z)]

HO basis space (configurations)

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

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

- 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

U.S. DEPARTMENT OF ENERGY | Office of Science

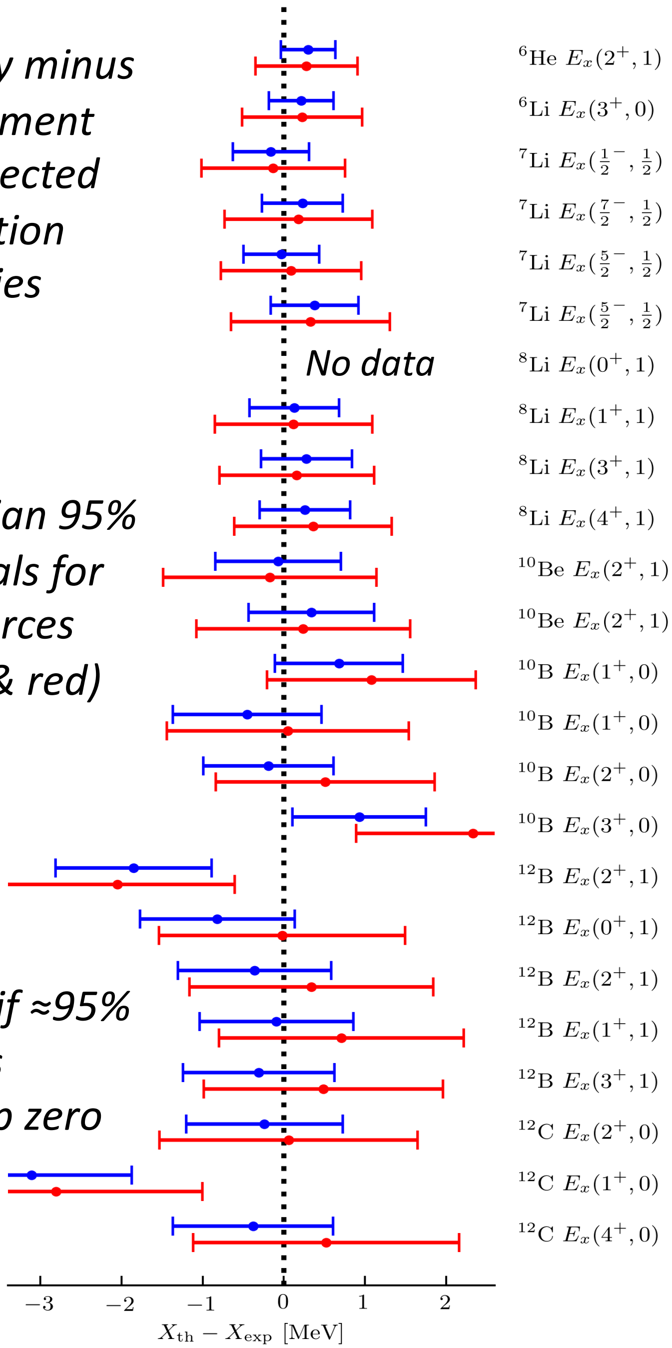
Excitation energies from effective field theory with quantified uncertainties

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]

Daejeon16 NN interaction

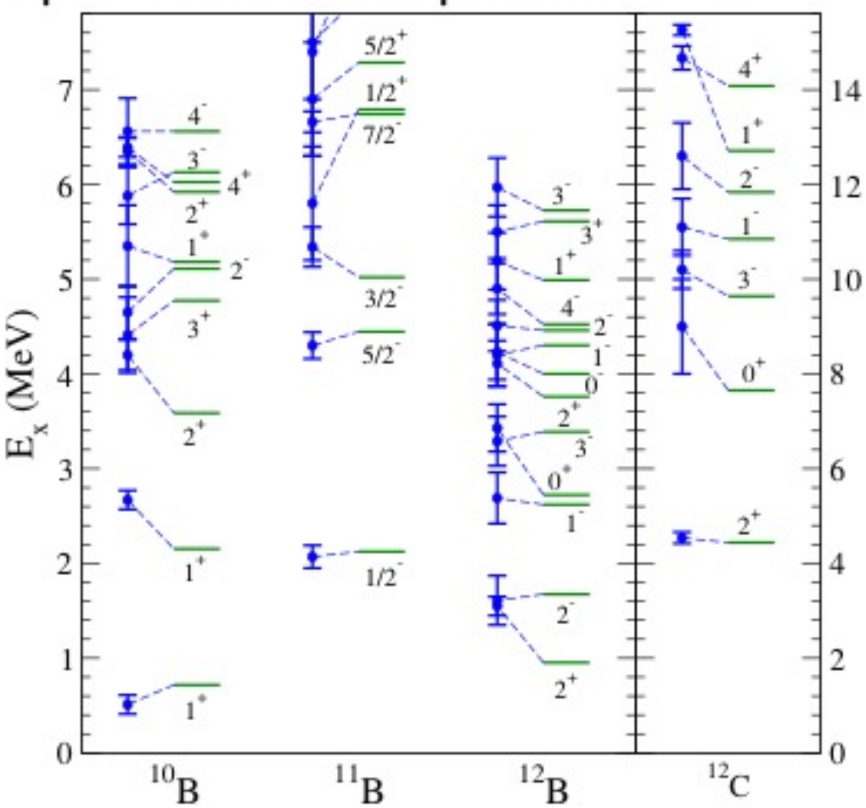
Based on SRG evolution of Entem-Machleidt "500" chiral N3LO to $\lambda = 1.5\ \mathrm{fm}^{-1}$ followed by Phase-Equivalent Transformations (PETs) to fit selected properties of light nuclei.

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

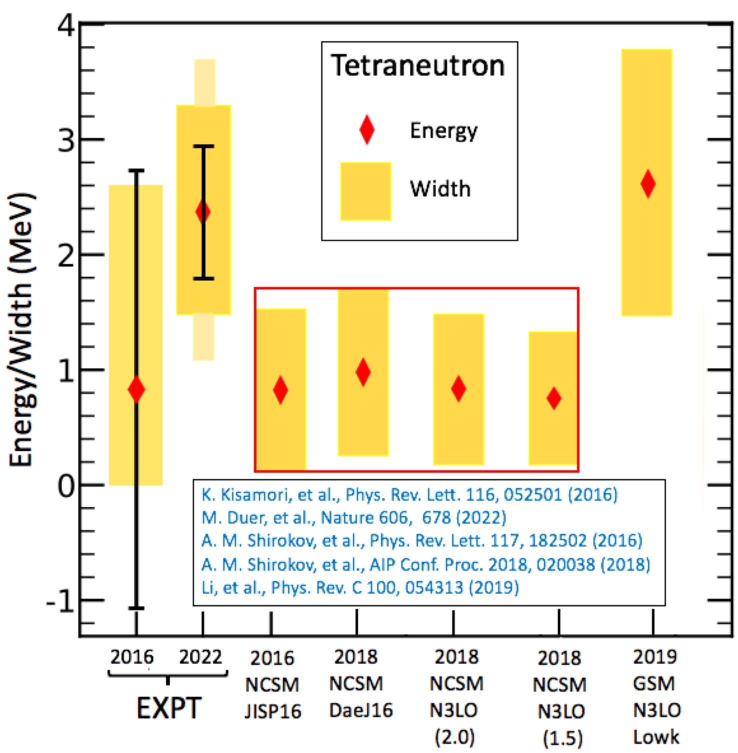


- difference of extrapolated E_b
- extrapolation uncertainties: max of E_b uncertainties
- good agreement with positive and negative parity spectra
- need large bases for 'intruder' and 'non-normal parity' states
- spectrum ^{10}B
  - correct gs 3^+ and excited 1^+
  - third 1^+ 'intruder' state
- excited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

Tetraneutron discovery confirms prediction

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)

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

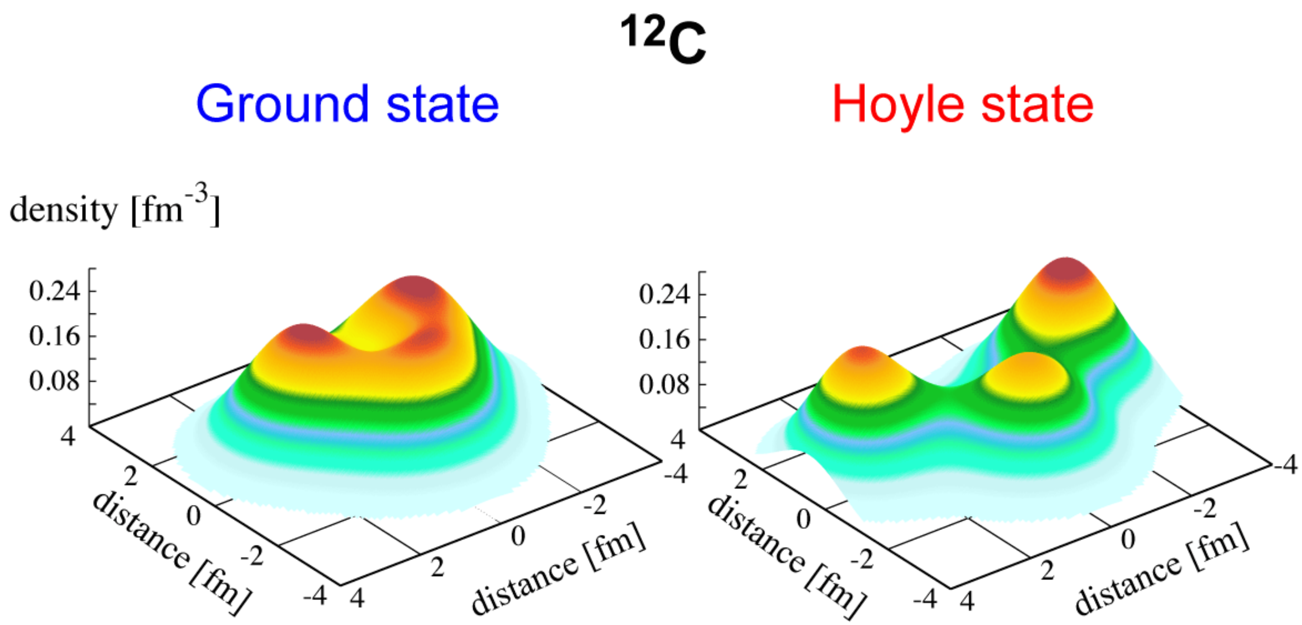
Objectives

- *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.

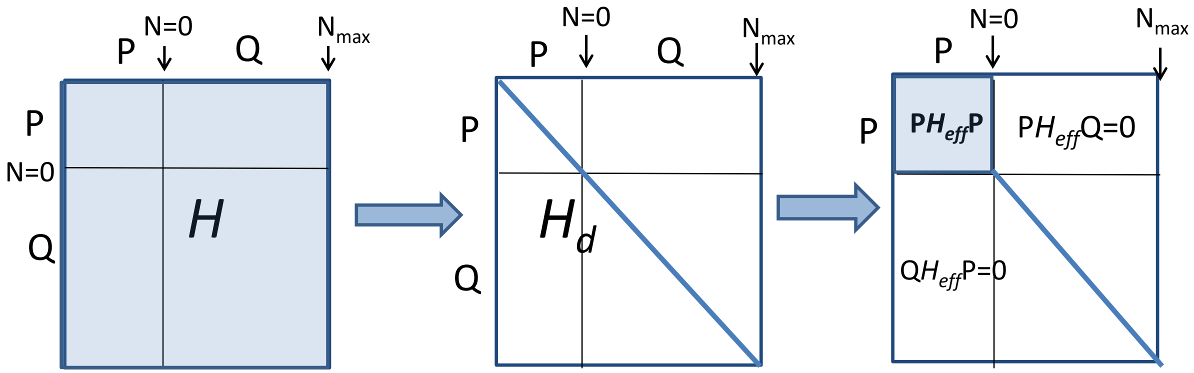


Accomplishments

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)

Ab-initio effective interaction from the NCSM

Okubo-Lee-Suzuki (OLS) similarity transformation
of the NCSM solution



$$H_d = UHU^\dagger \qquad H_{eff} = \frac{U_P^\dagger}{\sqrt{U_P U_P^\dagger}} H_d \frac{U_P}{\sqrt{U_P U_P^\dagger}}$$

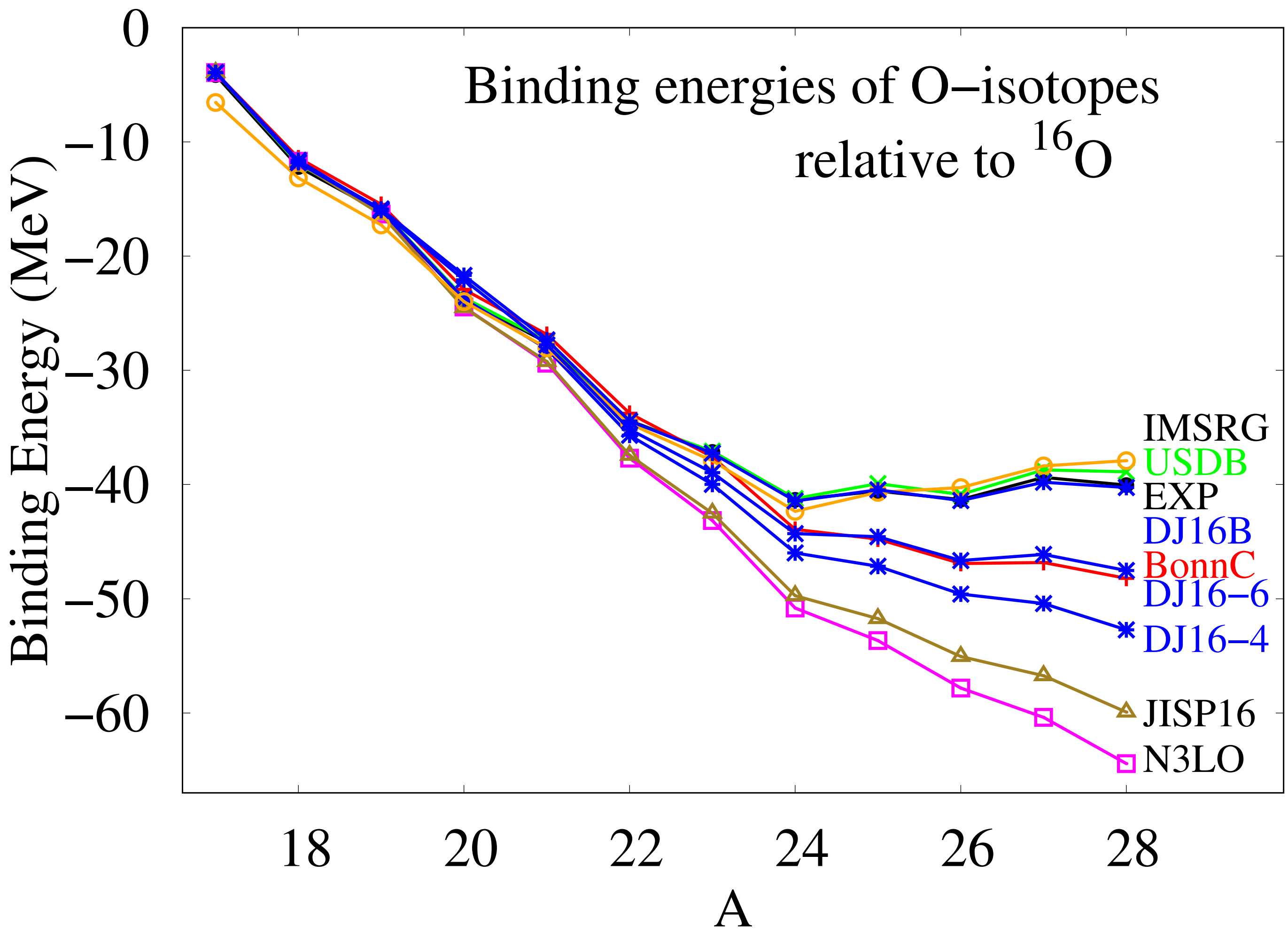
Flow

- NCSM for ^{18}F at $N_{\max}$
- H_{eff} for ^{18}F at $N = 0$ (OLS)
- ^{16}O at $N_{\max}$ (core energy)
- ^{17}O, ^{17}F at $N_{\max}$ (one-body terms)
- ϵ_j, $\langle ij|V_{\rm eff}|kl\rangle_{JT}$

Okubo, Progr. Theor. Phys. 12 (1954); Suzuki, Lee, Prog. Theor. Phys. 68 (1980)
Dikmen, Lisetskiy, Barrett, Maris, Shirokov, Vary, PRC91, 064301 (2015)
Vary, Basili, Du, Lockner, Maris, Pal, Sarker, PRC98, 065502 (2018)
Smirnova, Barrett, Kim, Shin, Shirokov, Dikmen, Maris, Vary, PRC100, 054329 (2019)
Shin, Smirnova, Shirokov, Yang, Barrett, Li, Kim, Maris and Vary, in preparation

Binding energies of O-isotopes

rms(DJ16-6) ≈ 3671 keV;   rms(DJ16B) ≈ 235 keV; rms(USDB) ≈ 467 keV



Scattering with the time-dependent basis function (tBF) approach

1. *Ab initio* structure calculation

$$H_0|\beta_i\rangle = E_i|\beta_i\rangle$$

$$H_0 = T_{rel} + V$$

⇓

$$\{|\beta_1\rangle, |\beta_2\rangle, \cdots, |\beta_n\rangle\}$$

2. Time-dependent

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

$$H(t) = T_{rel} + V + V_I(t)$$

⇓

- State vector becomes amplitudes
- Operators become matrices

- Natural extension of the NCSM
- Non perturbative
- *Ab initio*
- Full quantal coherence

$V_I(t)$

- Weijie Du, Peng Yin, Yang Li, Guangyao Chen, Wei Zuo, Xingbo Zhao, and James P. Vary, *Phys. Rev. C* **97**, 064620 (2018);
- Weijie Du, Peng Yin, Guangyao Chen, Xingbo Zhao, and James P. Vary, *in Proceedings of the International Conference "Nuclear Theory in the Supercomputing Era–2016" (NTSE-2016), Khabarovsk, Russia, September 19–23,* 2016.
- Peng Yin, Weijie Du, Wei Zuo, Xingbo Zhao and James P. Vary, J. Phys. G Nucl. Part. Phys. 49, 125102 (2022); & in prep.

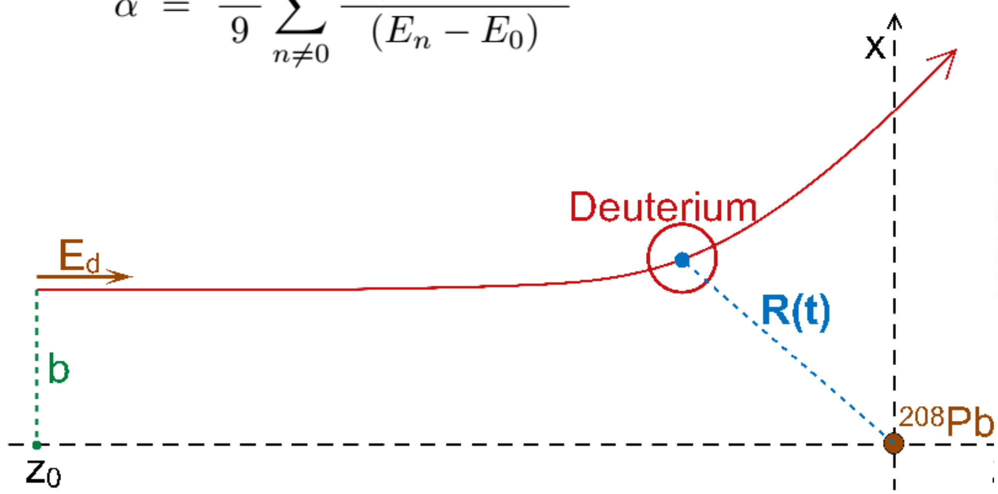
d+^{208}Pb scattering below Coulomb barrier
tBF with no adjustable parameters

Solve EOM for CM motion in external field:

$$V_{\text{pot}} = V_{\text{c}} + V_{\text{pol}}$$

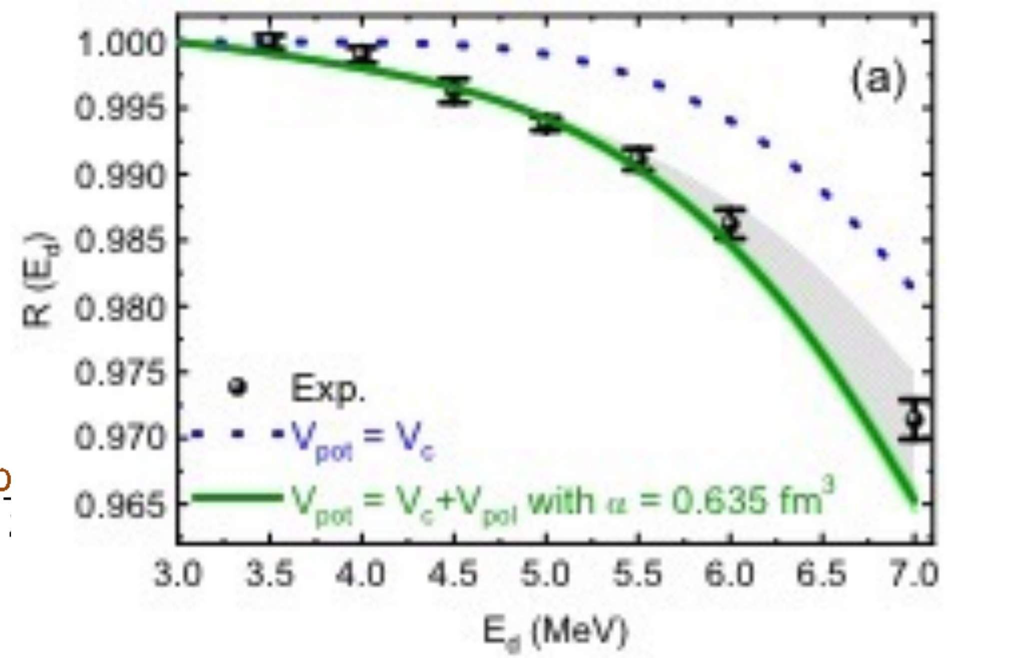
$$V_{pol} = -\frac{1}{2}\alpha Z^2 e^2 \frac{1}{(r^2 + r_0^2)^2}$$

$$\alpha = \frac{8\pi}{9} \sum_{n \neq 0} \frac{B(E1; 0 \to n)}{(E_n - E_0)}$$



$V_I(t)$ = time-dependent electric dipole field acting on np relative coordinates

$$R(E_d) = \frac{\sigma(E_d = 3\ \text{MeV}, \theta_1 = 60^\circ)}{\sigma(E_d = 3\ \text{MeV}, \theta_2 = 150^\circ)} \frac{\sigma(E_d, \theta_2 = 150^\circ)}{\sigma(E_d, \theta_1 = 60^\circ)}$$



- Scattering states of *np* system: LENPIC N4LO in 3DHO basis with large N_{max}
- Rutherford + polarization potential trajectory of CM
- Scattering basis space: coherent superposition of hundreds of states
- E1 transition included; M1 transitions found to be very weak in comparison

Peng Yin, Weijie Du, Wei Zuo, Xingbo Zhao and James P. Vary, J. Phys. G Nucl. Part. Phys. 49 125102 (2022)

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

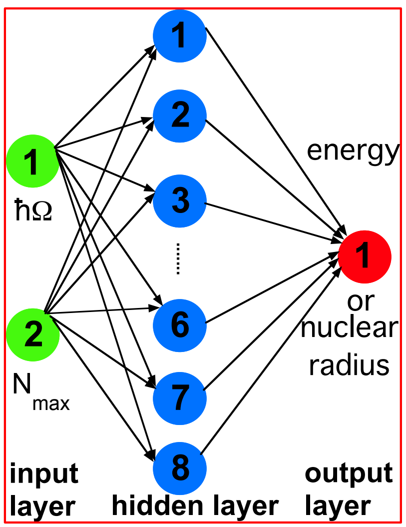
Deep Learning for Nuclear Binding Energy and Radius

Scientific Achievement

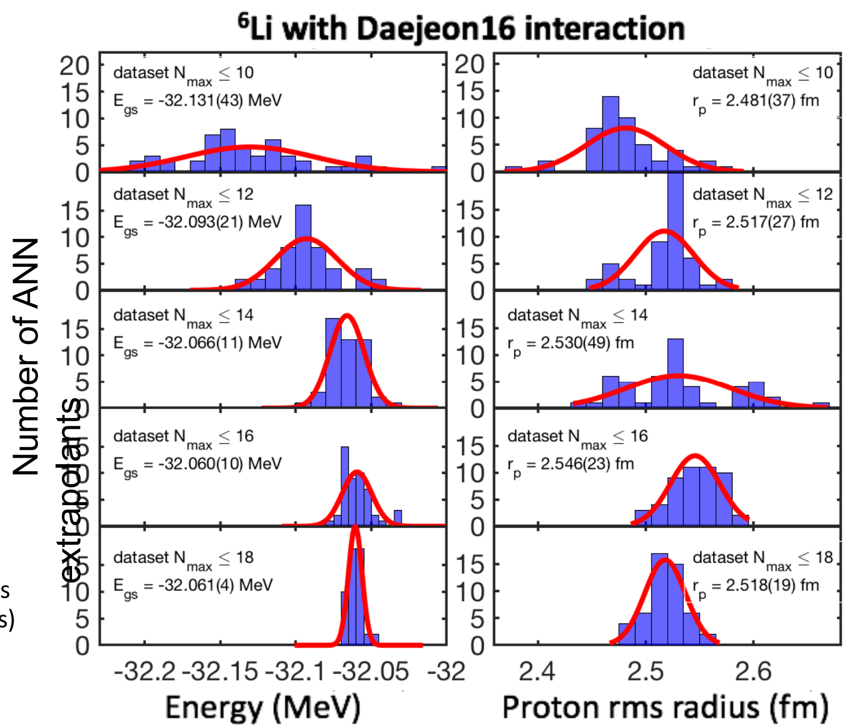
- Developed artificial neural networks (ANNs) for extending the application range of the *ab initio* No-Core Shell Model (NCSM)
- Demonstrated predictive power of ANNs for converged solutions of weakly converging simulations of the nuclear radius
- Provided a new paradigm for matching deep learning with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

Formulating the BLFQ problem on qubits

- Follows application of BLFQ-NJL model on quantum computers [Kreshchuk, 2009.07885]
- Here we adopt the Hamiltonian used in another previous work: [Qian, 2005.13806]

$$H_{\text{eff},\gamma_5} = \overbrace{\underbrace{\frac{\mathbf{k}_\perp^2 + m_q^2}{x} + \frac{\mathbf{k}_\perp^2 + m_{\bar{q}}^2}{1-x}}_{\text{LF kinetic energy}} + \underbrace{\kappa^4 x(1-x)\mathbf{r}_\perp^2 - \frac{\kappa^4}{(m_q+m_{\bar{q}})^2}\frac{\partial}{\partial x}\left(x(1-x)\frac{\partial}{\partial x}\right)}_{\text{confinement}} + V_g}^{H_{\text{eff}}} + H_{\gamma_5}$$

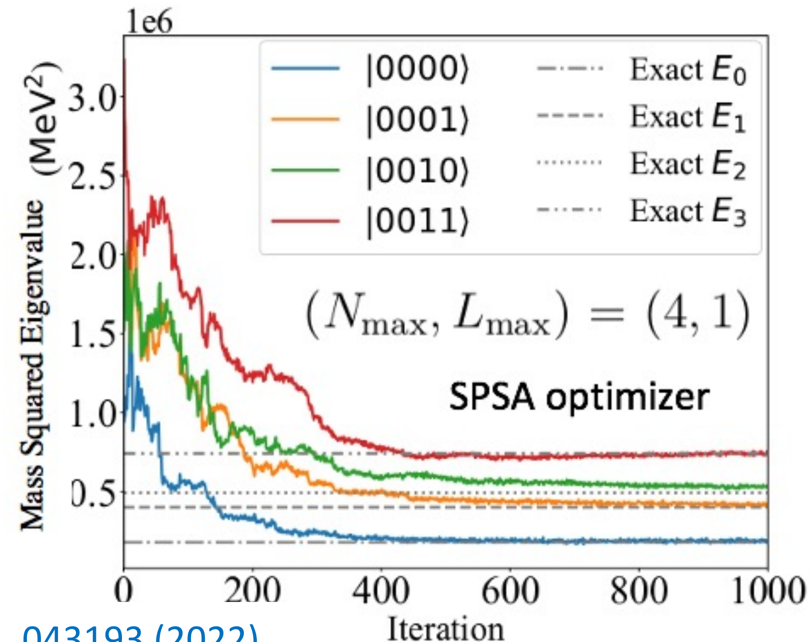
- Basis representation (BLFQ) is key to represent the Hamiltonian on qubits
- Small-size Hamiltonians (4-by-4 and 16-by-16) are used [Seeley, 1208.5986]
- Direct encoding and compact encoding are compared [Kreshchuk, 2002.04016]
- With evolved states: decay constants, PDFs, transition amplitudes, . . .

More qubits, less circuit depth (4-by-4 case):

$$\begin{aligned} H_{\text{direct}} = {} & 2269462\,\text{IIII} - 284243\,(\text{ZIII} + \text{IIZI}) \\ & - 850488\,(\text{IZII} + \text{IIIZ}) + 12714\,(\text{XZXI} + \text{YZYI}) \\ & - 7883\,(\text{IXZX} + \text{IYZY}), \end{aligned}$$

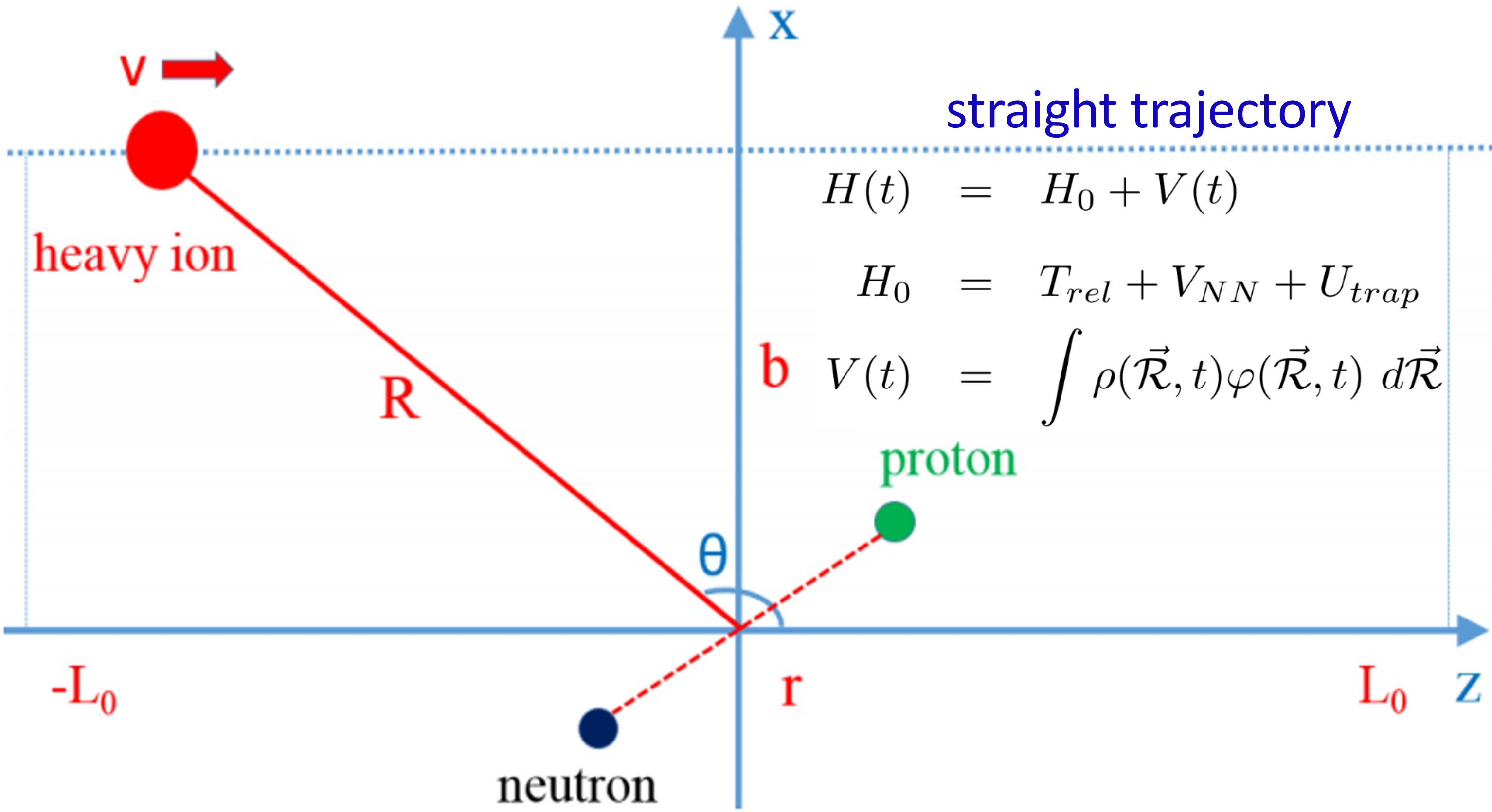
Fewer qubits, greater circuit depth (4-by-4 case):

$$\begin{aligned} H_{\text{compact}} = {} & 1134731\,\text{II} - 566245\,\text{IZ} \\ & + 4831\,\text{XI} + 20598\,\text{XZ} \end{aligned}$$



W. Qian, R. Basili, S. Pal, G.R. Luecke and J.P. Vary, Phys. Rev. Research 4, 043193 (2022)

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



$$H(t) = H_0 + V(t)$$

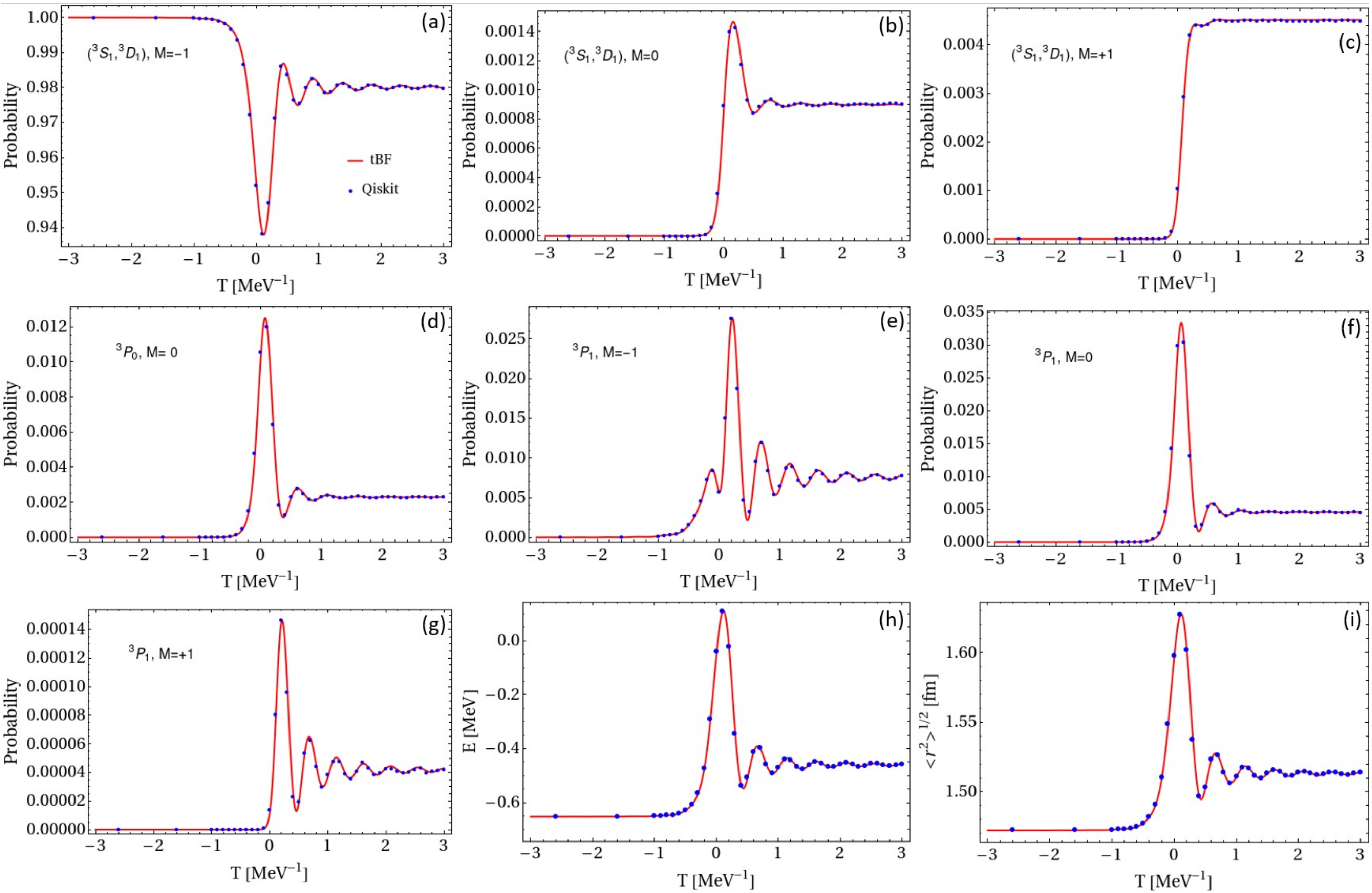
$$H_0 = T_{rel} + V_{NN} + U_{trap}$$

$$V(t) = \int \rho(\vec{\mathcal{R}}, t)\varphi(\vec{\mathcal{R}}, t)\, d\vec{\mathcal{R}}$$

- 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)

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