

# Nuclear Structure Across Energy Scales

James P. Vary  
Iowa State University

Nucleus-2022

Moscow  
July 11-16, 2022

## The Overarching Questions

- How did visible matter come into being and how does it evolve?
- How does subatomic matter organize itself and what phenomena emerge?
- Are the fundamental interactions that are basic to the structure of matter fully understood?
- How can the knowledge and technological progress provided by nuclear physics best be used to benefit society?

- *NRC Decadal Study*

## The Time Scale

- Protons and neutrons formed  $10^{-6}$  to 1 second after Big Bang (13.7 billion years ago)
- H, D, He, Li, Be, B formed 3-20 minutes after Big Bang
- Other elements born over the next 13.7 billion years

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?

Degrees of Freedom

## Heirarchy of first principles problems

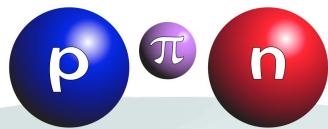
Physics of Hadrons



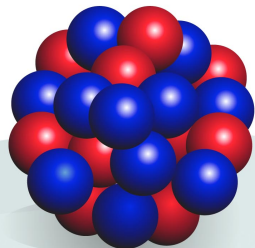
Energy (MeV)  
> 1000



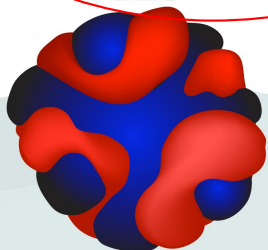
940  
neutron mass



140  
pion mass



8  
proton separation  
energy in lead



1.12  
vibrational  
state in tin



0.043  
rotational  
state in uranium

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

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 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



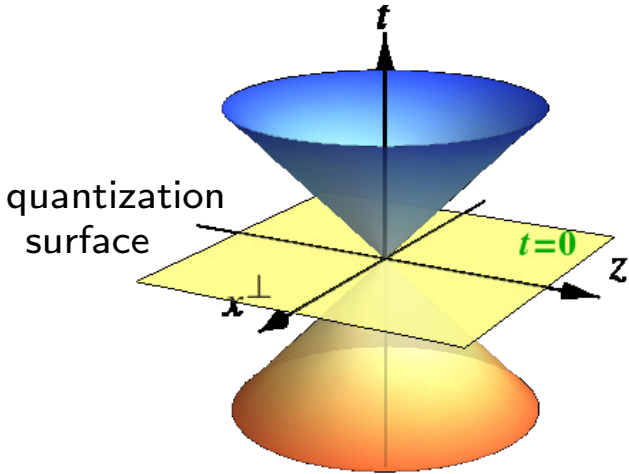
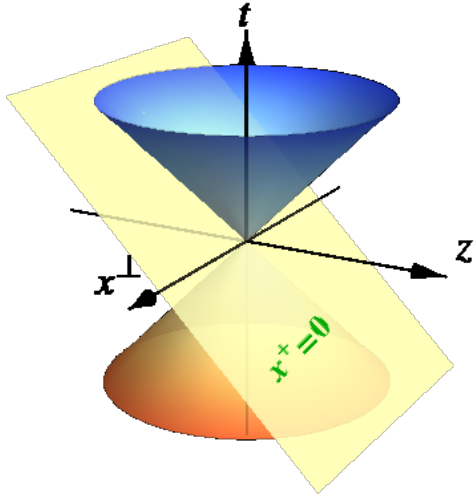
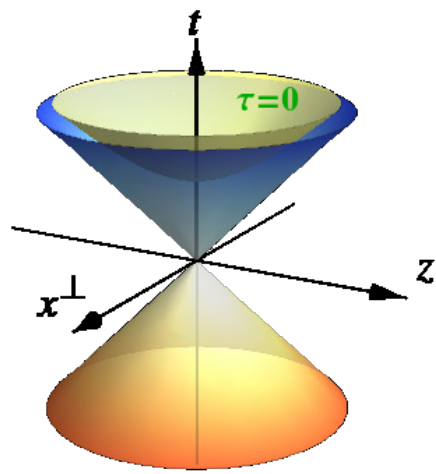
Dirac's forms of relativistic dynamics [Dirac, Rev. Mod. Phys. **21**, 392 1949]

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

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

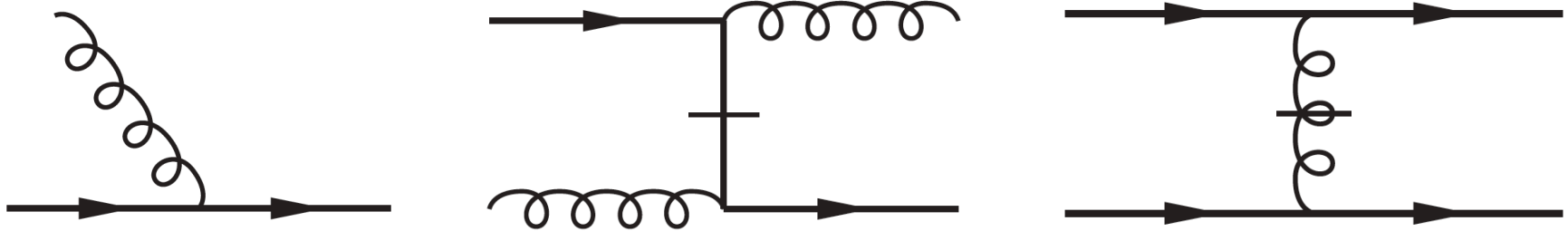
Front form defines relativistic dynamics on the light front (LF):  $x^+ = x^0 + x^3 = t + z = 0$

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

	instant form	front form	point form
time variable	$t = x^0$	$x^+ \triangleq x^0 + x^3$	$\tau \triangleq \sqrt{t^2 - \vec{x}^2 - a^2}$
			
Hamiltonian	$H = P^0$	$P^- \triangleq P^0 - P^3$	$P^\mu$
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	$p^0 = \sqrt{\vec{p}^2 + m^2}$	$p^- = (\vec{p}_\perp^2 + m^2)/p^+$	$p^\mu = mv^\mu \ (v^2 = 1)$

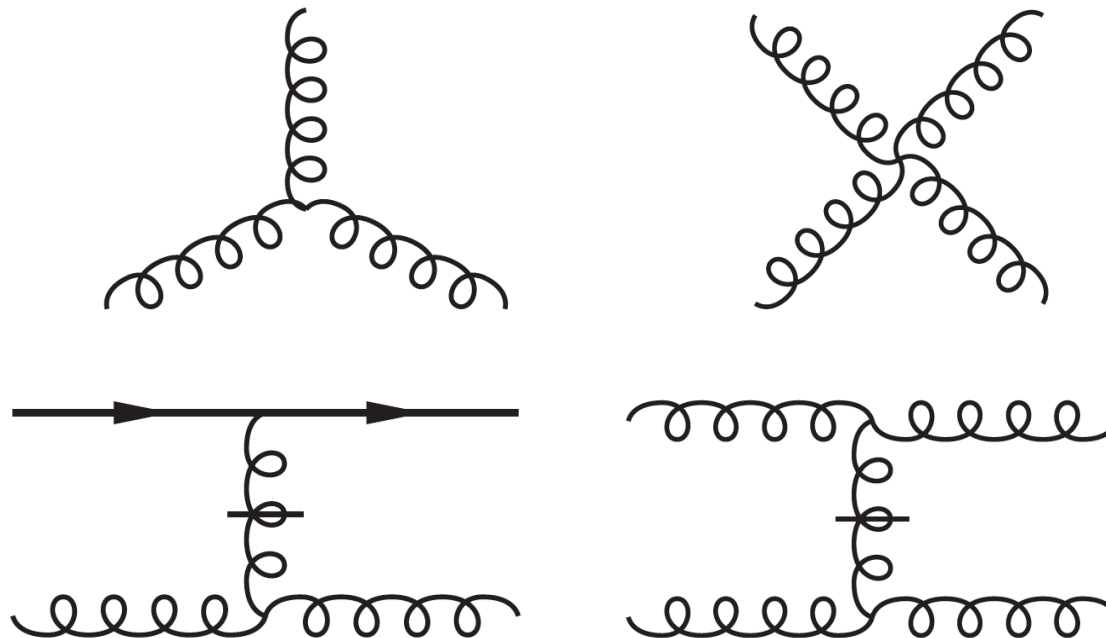


# Light Front (LF) Hamiltonian Defined by its Elementary Vertices in LF Gauge



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)]

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

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

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

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

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

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

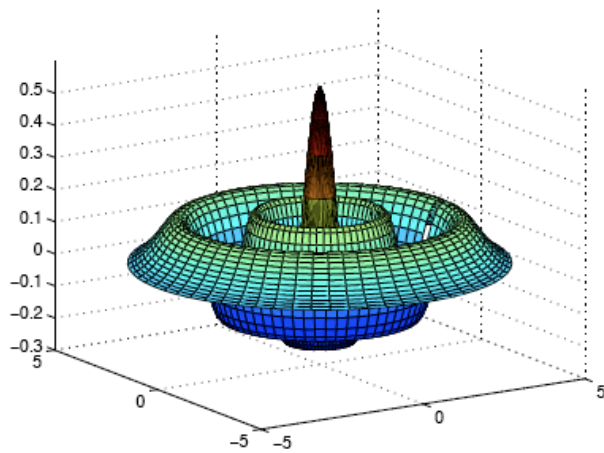
$$f_{\alpha=\{nml\}}(\vec{k}_\perp, x) = \phi_{nm}(\vec{k}_\perp / \sqrt{x(1-x)}) \chi_l(x)$$

$\phi_{nm}$  2D-HO functions as in AdS/QCD

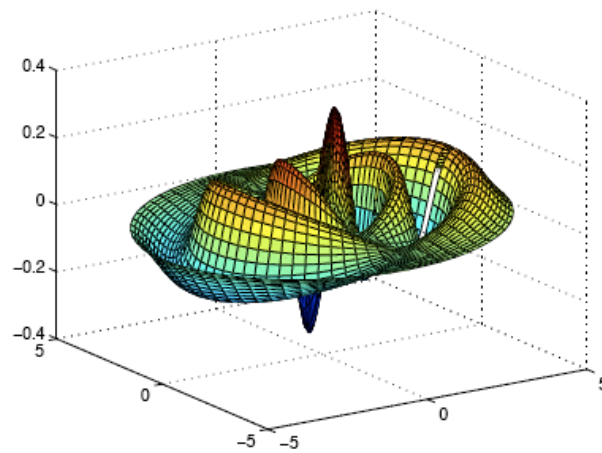
$\chi_l$  Jacobi polynomials times  $x^a(1-x)^b$

## Set of Transverse 2D HO Modes for $n=4$

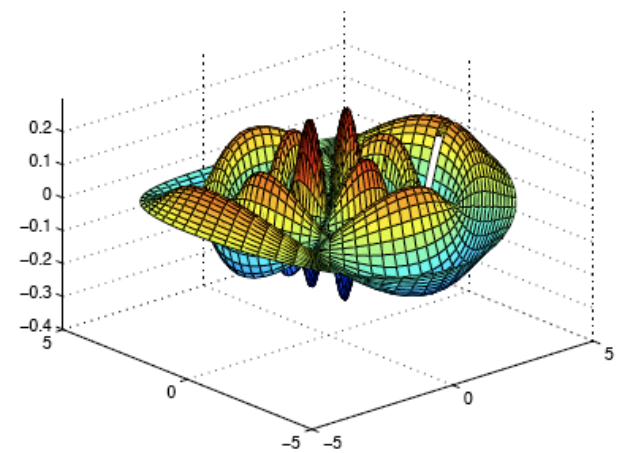
$m=0$



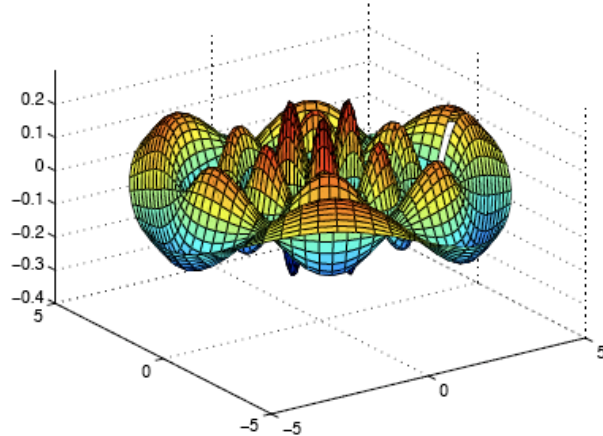
$m=1$



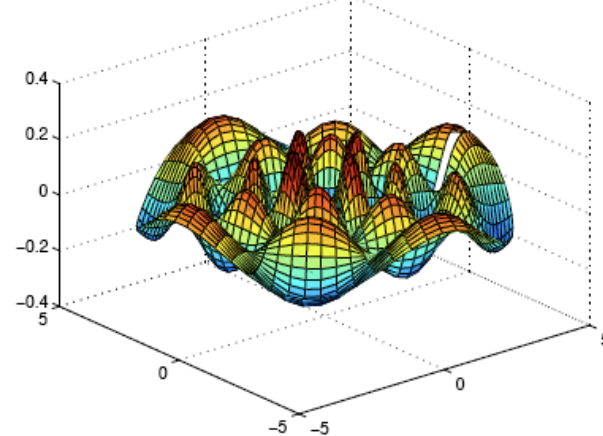
$m=2$



$m=3$



$m=4$



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)

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

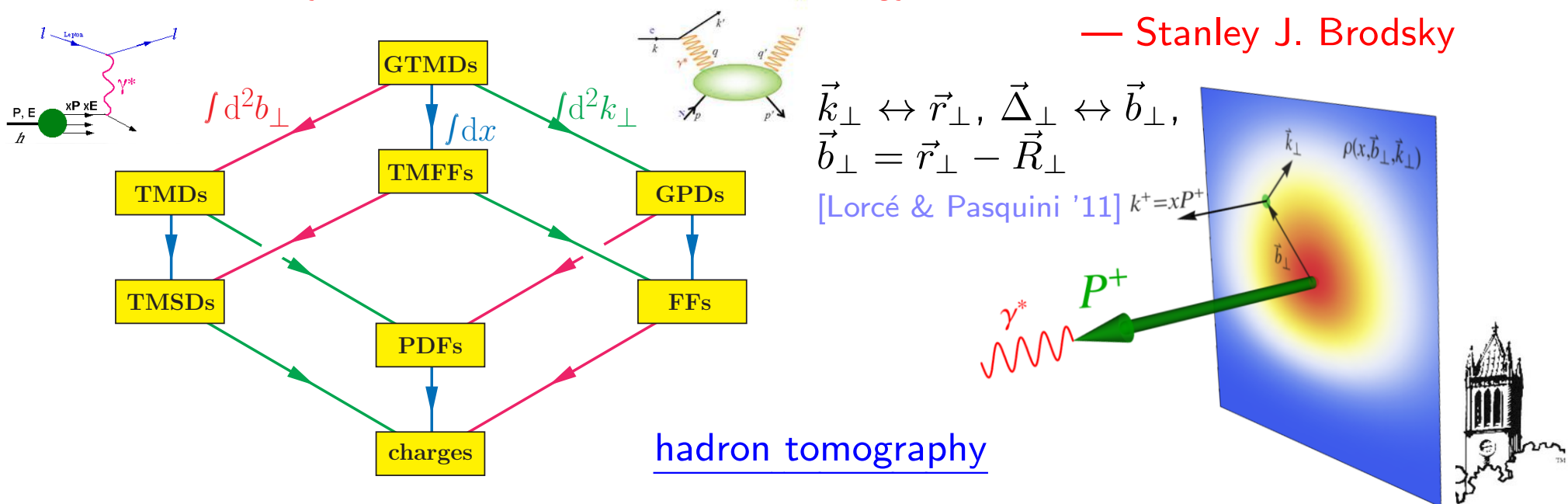
LFWFs are *frame-independent* (boost invariant) and depend only on the relative variables:  $x_i \equiv p_i^+ / P^+$ ,  $\vec{k}_{i\perp} \equiv \vec{p}_{i\perp} - x_i \vec{P}_\perp$

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



# Heavy Quarkonia

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

- The effective Hamiltonian:

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

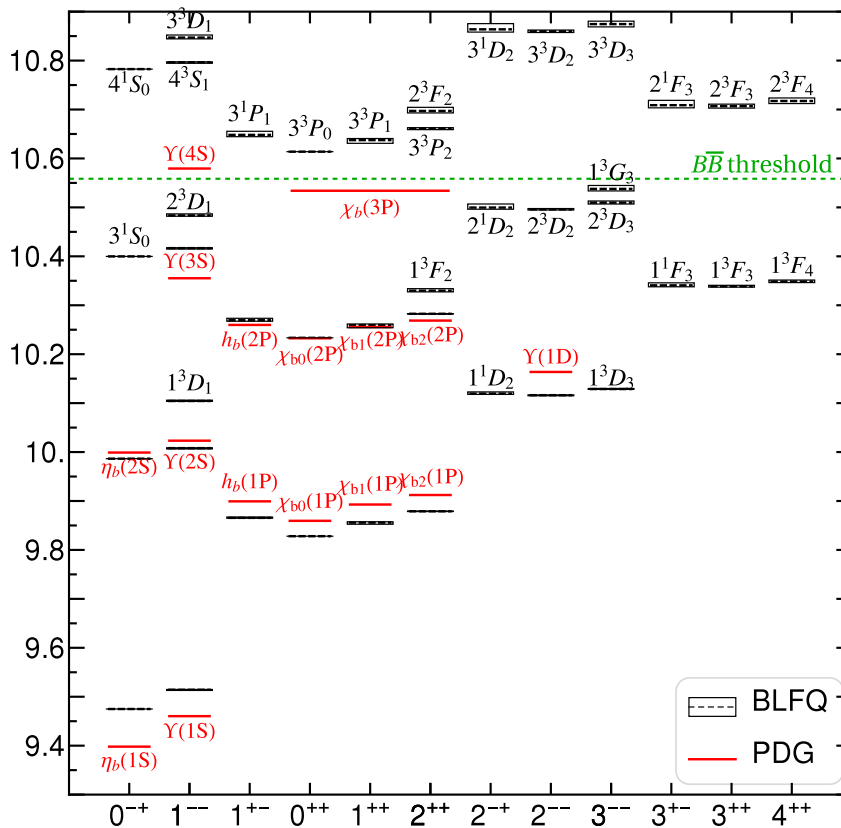
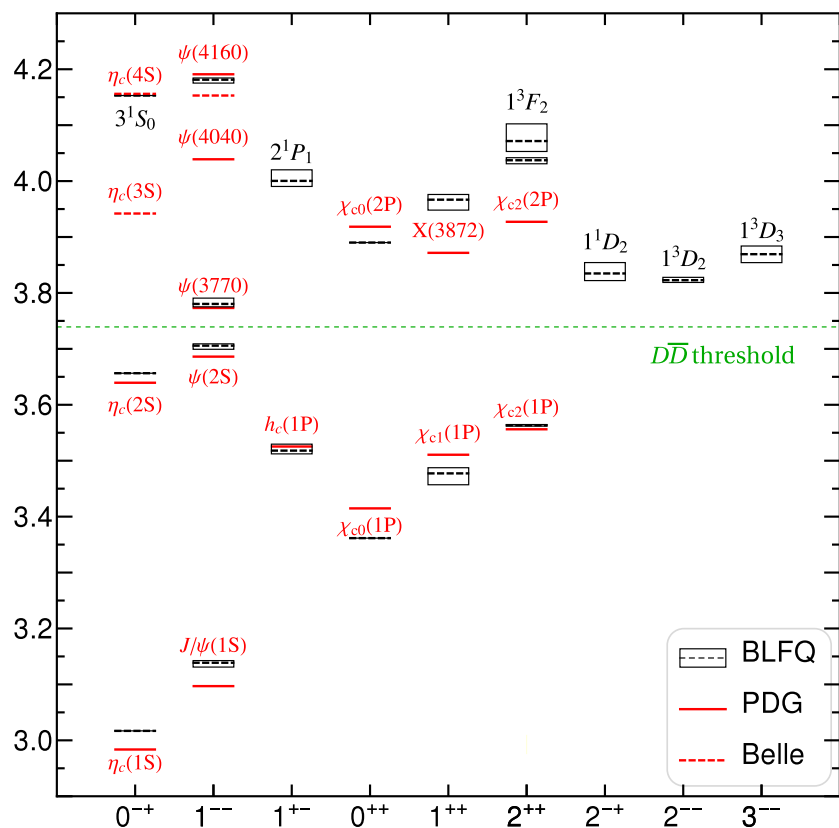
$H_0$

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
 
$$V_g = -\frac{4}{3} \frac{4\pi\alpha_s(Q^2)}{Q^2} \bar{u}_{\sigma'} \gamma^{\mu} u_{\sigma} \bar{v}_s \gamma_{\mu} v_{s'} \quad [\text{M.Krautgartner:PRD45,1992}]$$
- Basis representation
  - valence Fock sector:  $|q\bar{q}\rangle$
  - 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)]



	$\kappa$ (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

$\kappa$  determined from fits to spectrum follows the HQET trajectory  $\kappa_h \propto \sqrt{M_h}$ , in agreement with recent LFH result [Dosch et al, PRD95 (2017)]

[Dosch et al, PRD95 (2017)]

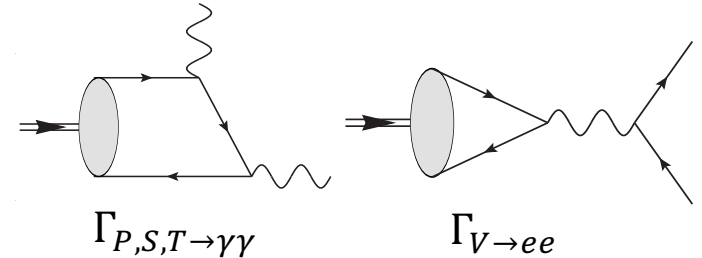




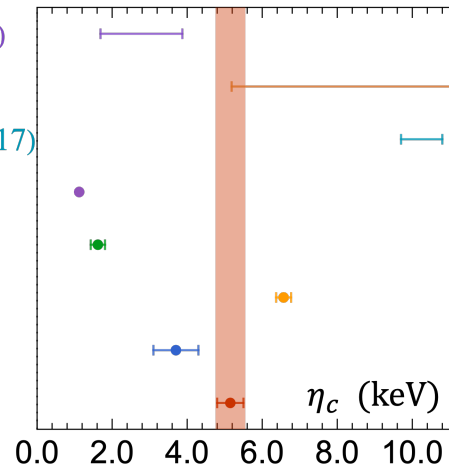
# Dilepton and Diphoton widths of charmonia in BLFQ

Y. Li, M. Li and J.P. Vary, Phys. Rev. D 105, L071901 (2022)

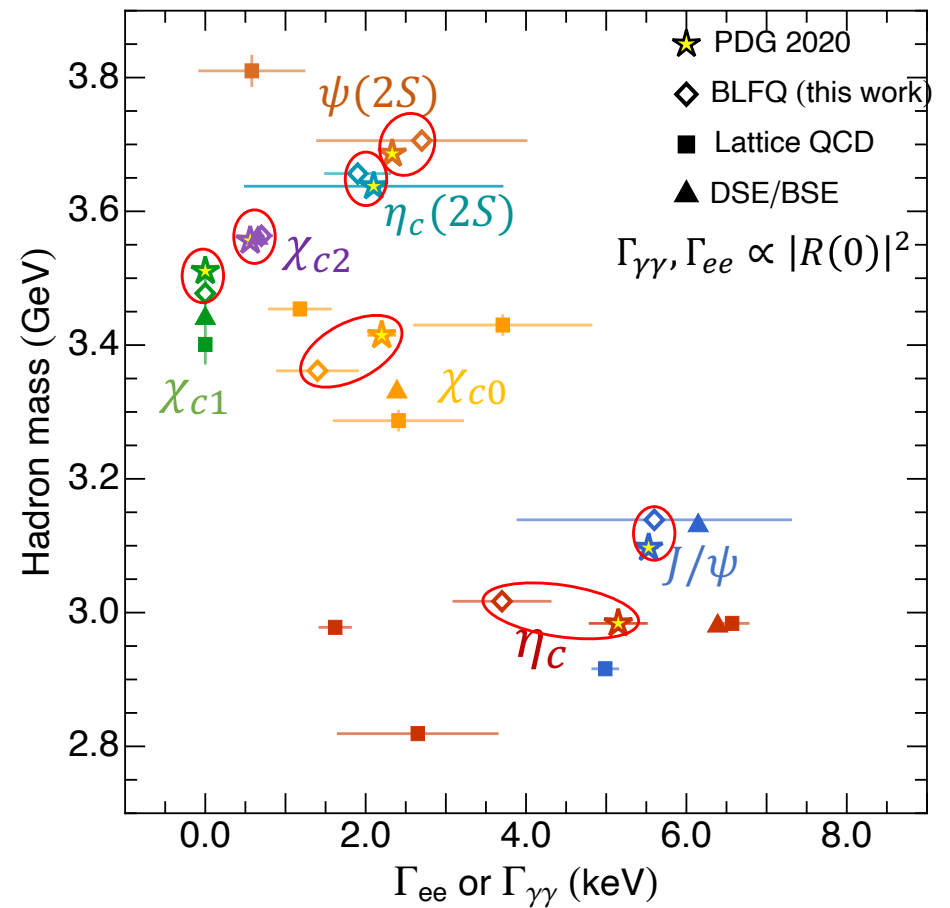
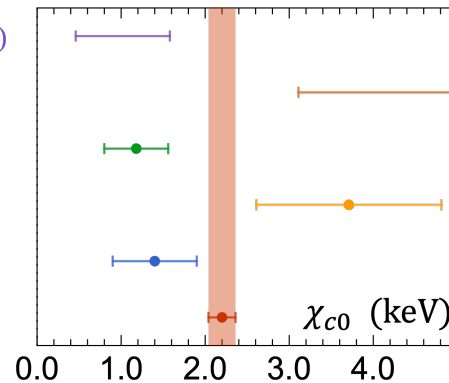
- ✓ Notoriously challenging
- ✓ BLFQ predictions are very competitive!
  - ✓ No parameters were adjusted!



NRQM/LF (Babiarz 2019)  
 NRQM (Babiarz 2019)  
 NNLO NRQCD (Feng 2017)  
 Lattice (Chen 2016)  
 Lattice (Chen 2020)  
 Lattice (Meng 2021)  
 BLFQ (this work)  
 PDG 2020



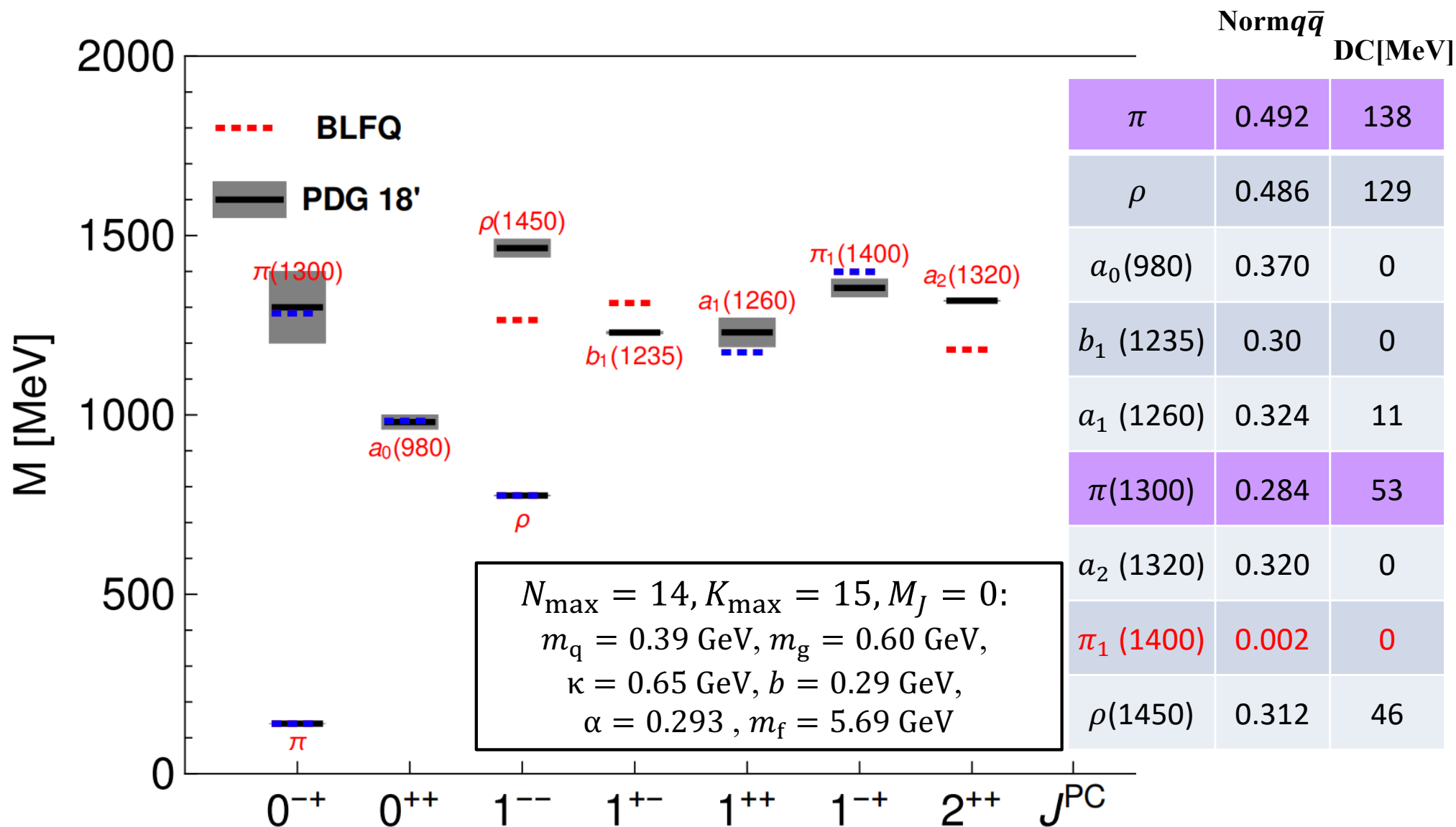
NRQM/LF (Babiarz 2019)  
 NRQM (Babiarz 2019)  
 Lattice (Chen 2020)  
 Lattice (Zou 2021)  
 BLFQ (this work)  
 PDG 2020



Lattice: Dudek '06, Chen '16, Chen '20, Meng '21, Zou '21;  
 DSE: Chen '17  
 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



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

Fix the parameters by fitting six blue states

- $\pi_1(1400)$ :  $|q\bar{q}g\rangle$  dominates
- $\pi(1300)$ : the DC is smaller than the DC of pion

# Light-Front Hamiltonian for Baryons

S. Xu, C. Mondal, J. Lan, X. Zhao, Y. Li and J.P. Vary, Phys. Rev. D 104, 094036 (2021); LC2021; & in preparation

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

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

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

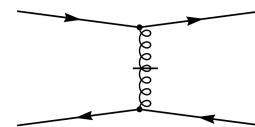
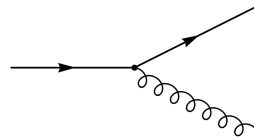
$$H_{longi} \sim - \sum_{ij} \kappa_L^4 \partial_{x_i} (x_i x_j \partial_{x_j}) \quad \text{---Y Li, X Zhao, P Maris, J Vary, PLB 758(2016)}$$

$$|P_{baryon}\rangle = |qqq\rangle + |qqqg\rangle + |qqq q\bar{q}\rangle + \dots$$

➤ Include the first and second Fock sector

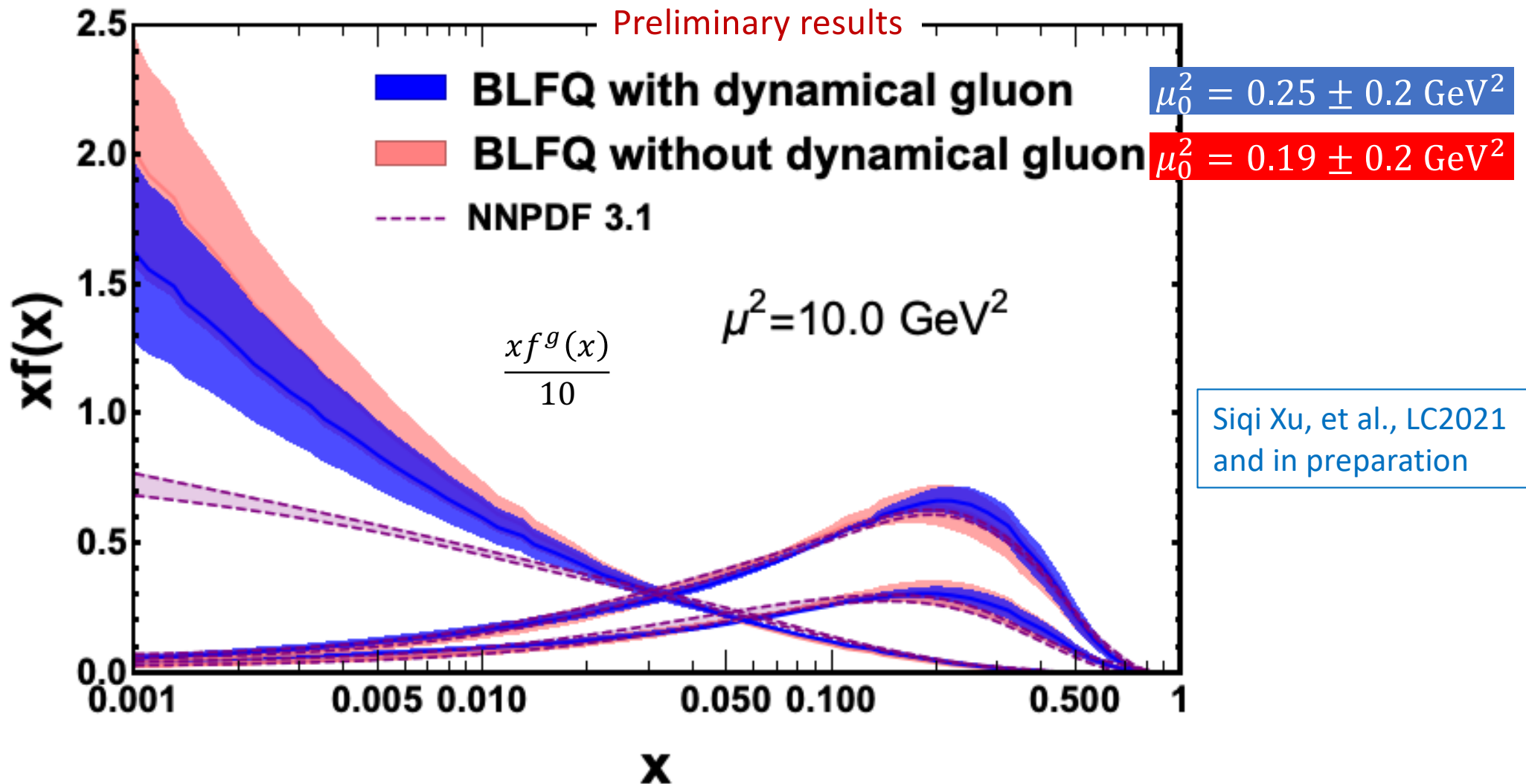
$$H_{Interact} = H_{Vertex} + H_{inst} = g \bar{\psi} \gamma^\mu T^a \psi A_\mu^a + \frac{g^2 C_F}{2} j^+ \frac{1}{(i\partial^+)^2} j^+$$

$$N_{\max} = 9, K = 16.5$$



$m_u$	$m_d$	$\kappa$	$m_g$	$m_{int}$	$b_{inst}$	$b$	$g$
0.35 GeV	0.3 GeV	0.54 GeV	0.5 GeV	1.9 GeV	3 GeV	0.65 GeV	2.2

# Unpolarized Parton Distribution Functions



Without second Fock sector  $|qqqg\rangle$ , the gluon is generated dynamically from the DGLAP evolution.

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



# 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,

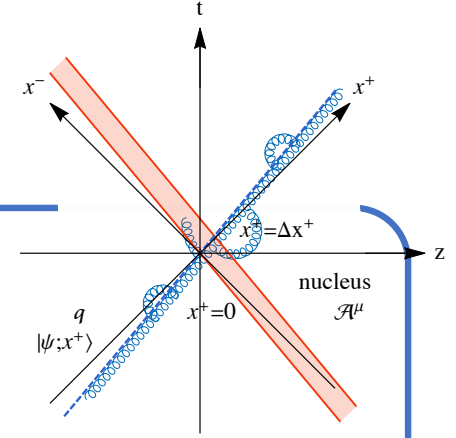
$$|\psi(x^+)\rangle = \mathcal{T}_+ \exp\left[-\frac{i}{2}\int_0^{x^+} dz^+ P^-(z^+)\right] |\psi(0)\rangle$$

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

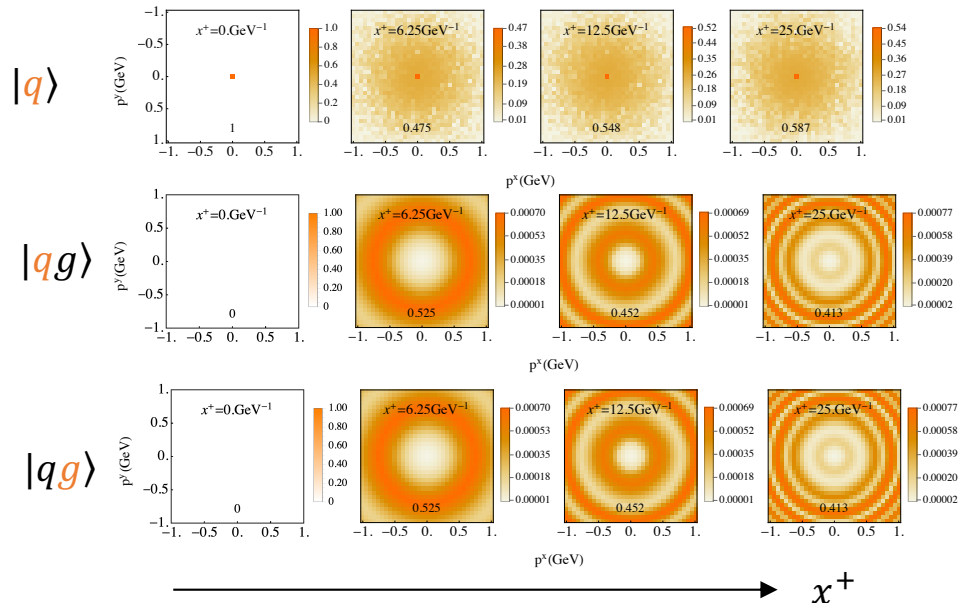
### ❖ Basis representation:

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*



## 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, arXiv:2203.14447
- 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

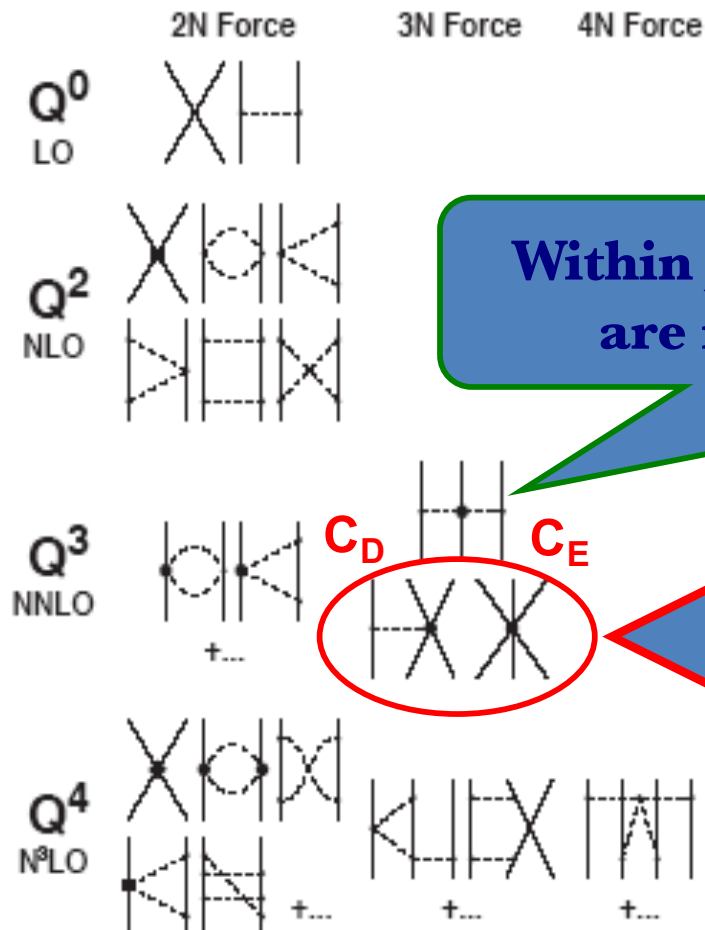
# Effective Nucleon Interaction

## (Chiral Perturbation Theory)

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

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

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



Within  $\chi$ PT  $2\pi$ -NNN Low Energy Constants (LEC) are related to the NN-interaction LECs  $\{c_i\}$ .

Terms suggested within the Chiral Perturbation Theory

**Regularization** is essential, which is 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

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

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

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

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

- 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,  $\alpha, \beta, \dots$
- 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  $[\alpha = (n, l, j, m_j, \tau_z)]$

$$\text{HO basis space (configurations)} \left\{ \begin{array}{l} |\Phi_n\rangle = [a_{\alpha}^+ \dots a_{\zeta}^+]_n |0\rangle \\ n = 1, 2, \dots, 10^{10} \text{ or more!} \end{array} \right.$$

- 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

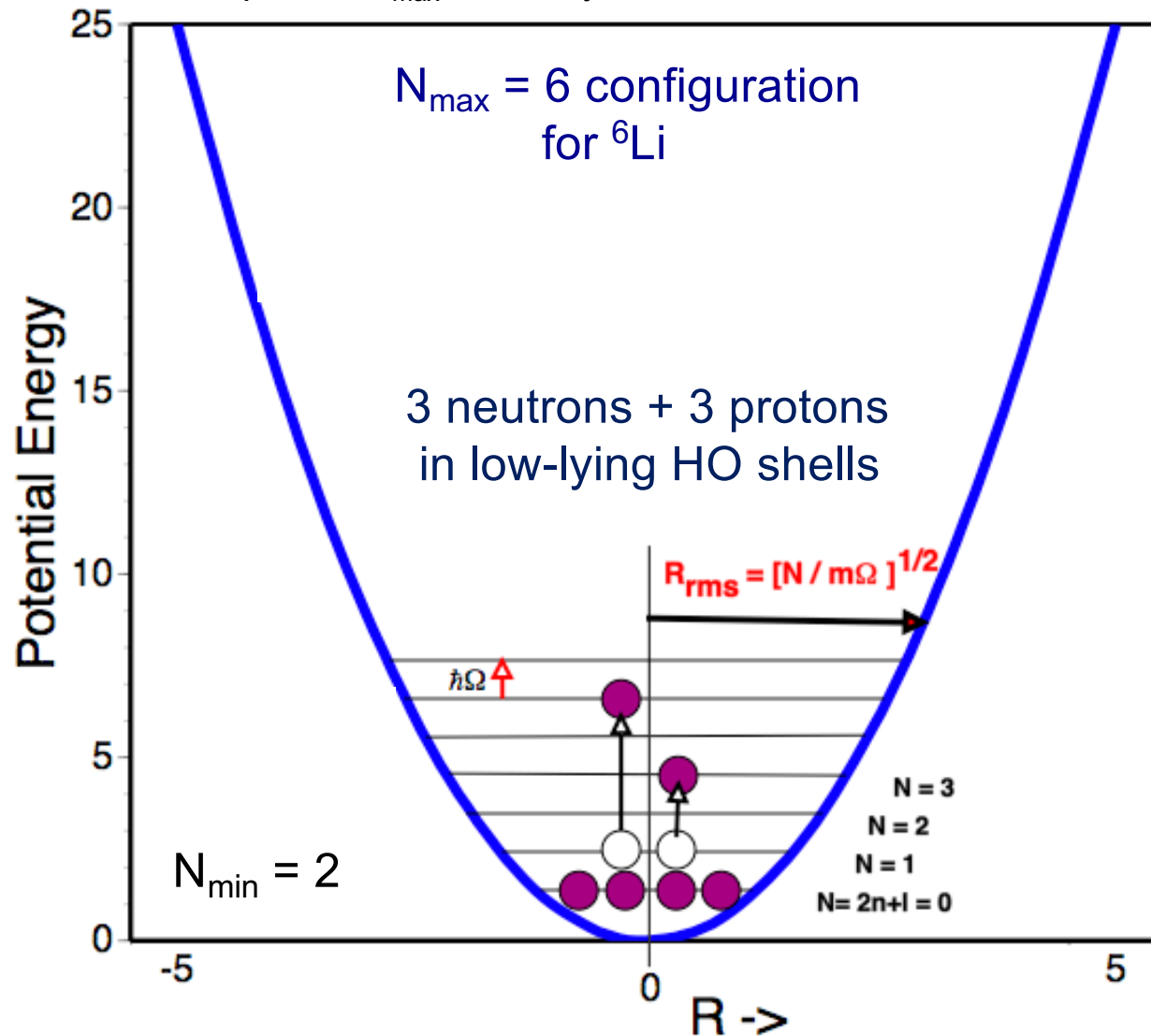


$N_{\min} \equiv$  HO quanta of lowest configuration

$N_{\max} \equiv$  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,  $M_J, \dots$ )

extrapolate:  $N_{\max} \rightarrow$  infinity



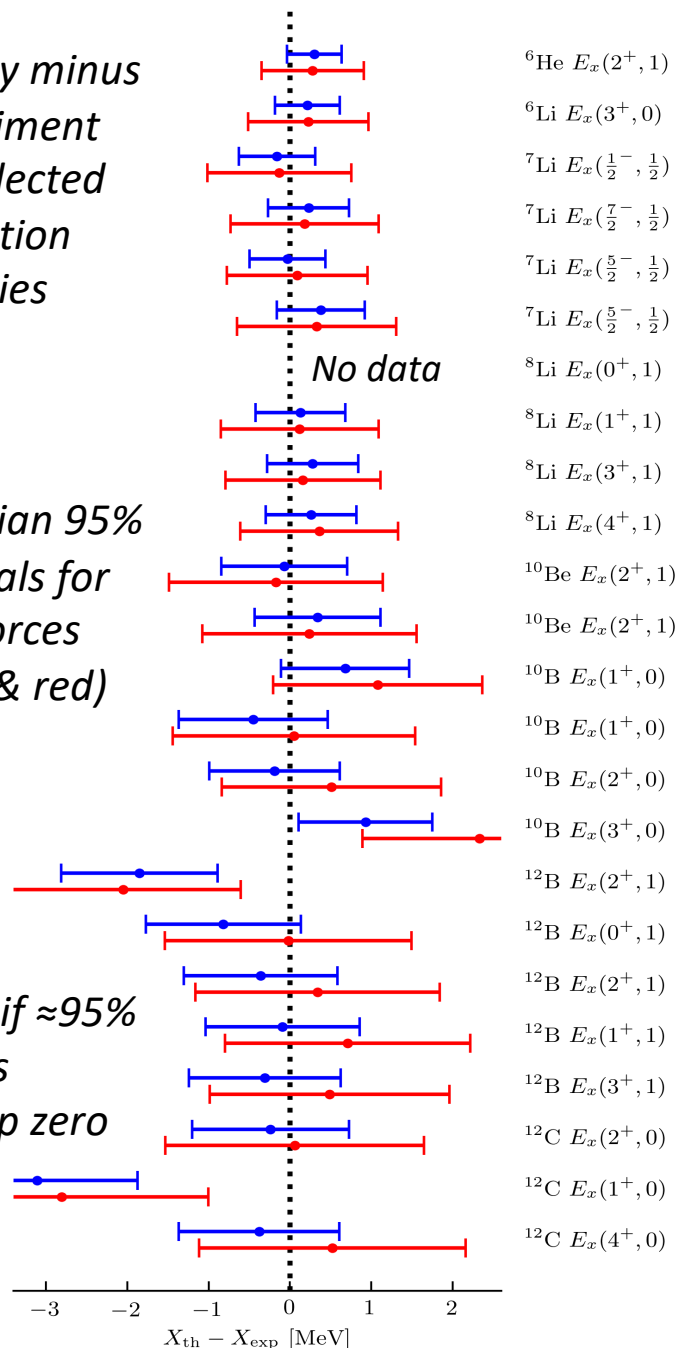


# Excitation energies from effective field theory with quantified uncertainties

Theory minus  
experiment  
for selected  
excitation  
energies

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

Check if  $\approx 95\%$   
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  $^{12}\text{C}$  and  $^{12}\text{B}$  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

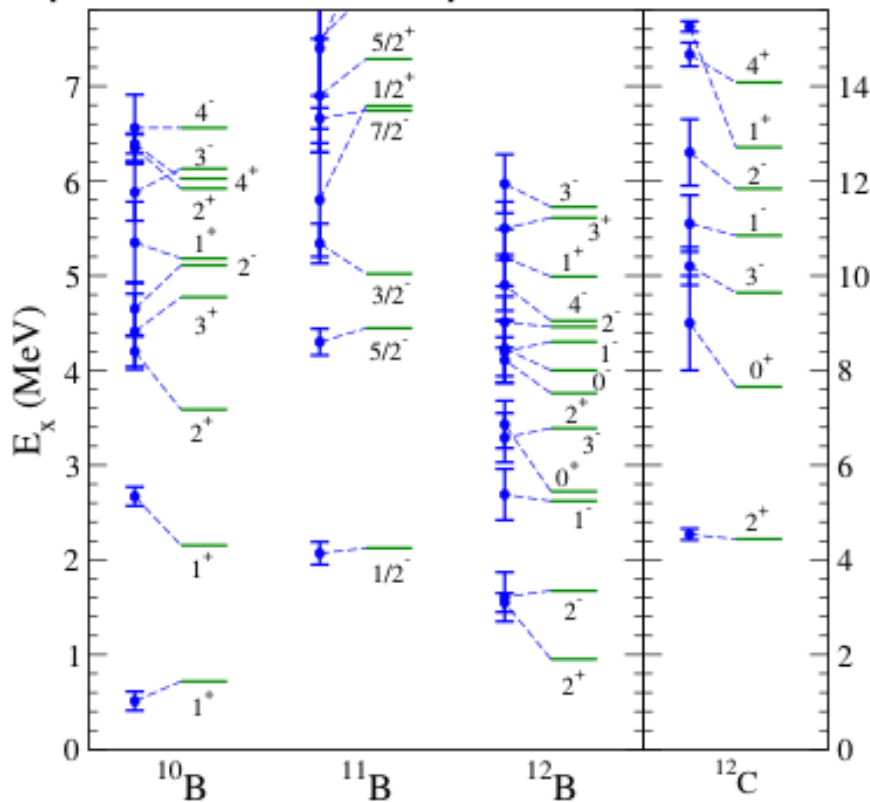
Based on SRG evolution of Entem-Machleidt “500” chiral N3LO to  $\lambda = 1.5 \text{ fm}^{-1}$  followed by Phase-Equivalent Transformations (PETs) to fit selected properties of light nuclei.

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 $^{12}\text{C}$

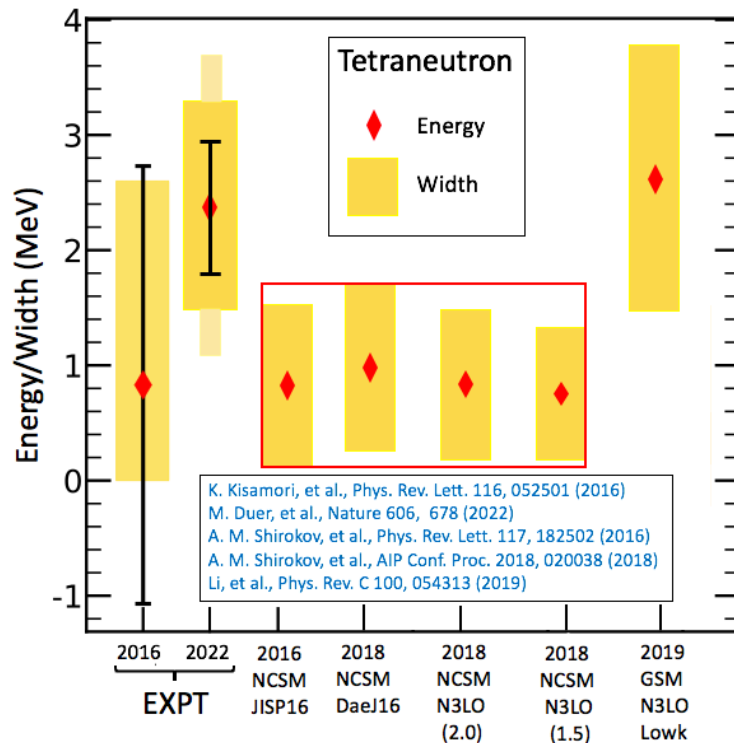


- ▶ difference of extrapolated  $E_b$
- ▶ extrapolation uncertainties:  
max of  $E_b$  uncertainties
- ▶ good agreement with positive  
and negative parity spectra
- ▶ need large bases for 'intruder'  
and 'non-normal parity' states
- ▶ spectrum  $^{10}\text{B}$ 
  - ▶ correct gs  $3^+$  and excited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

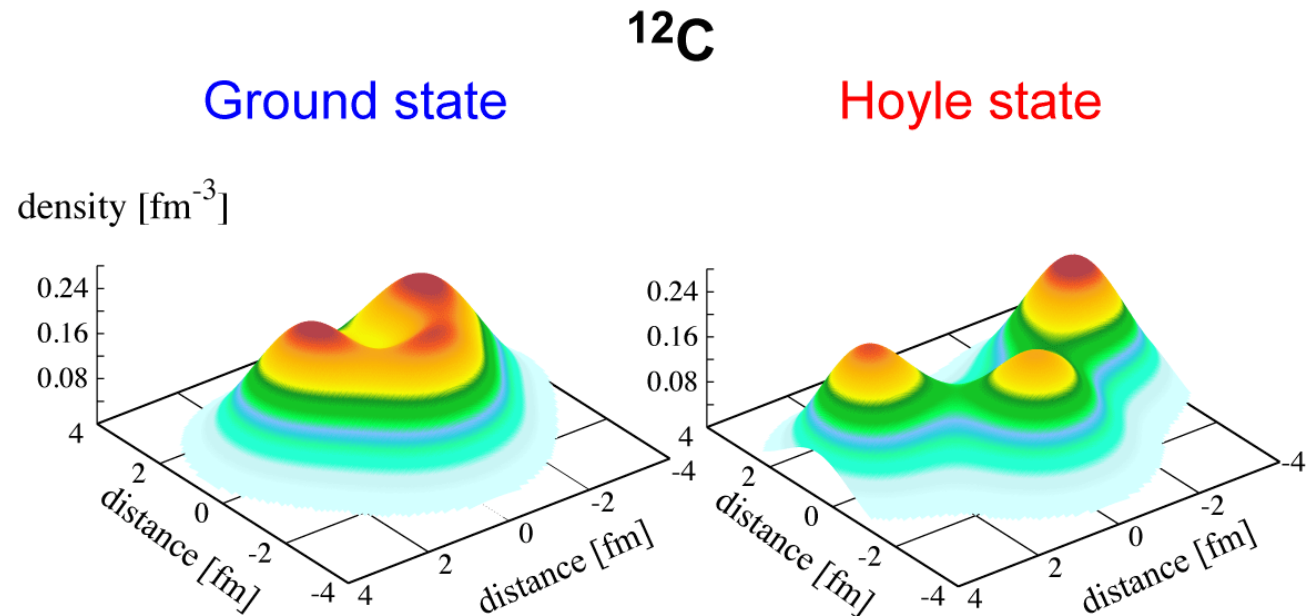
## Objectives

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

## 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  $^{12}\text{C}$ , 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  $^{12}\text{C}$  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.

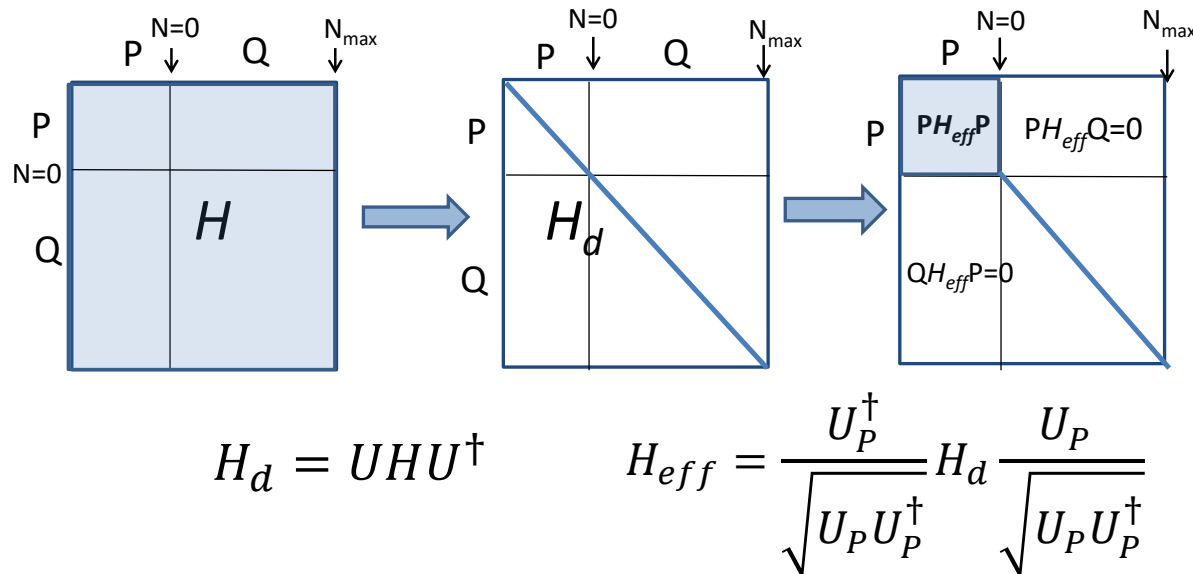


## Accomplishments

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



Flow

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

Okubo, *Progr. Theor. Phys.* 12 (1954); Suzuki, Lee, *Prog. Theor. Phys.* 68 (1980)

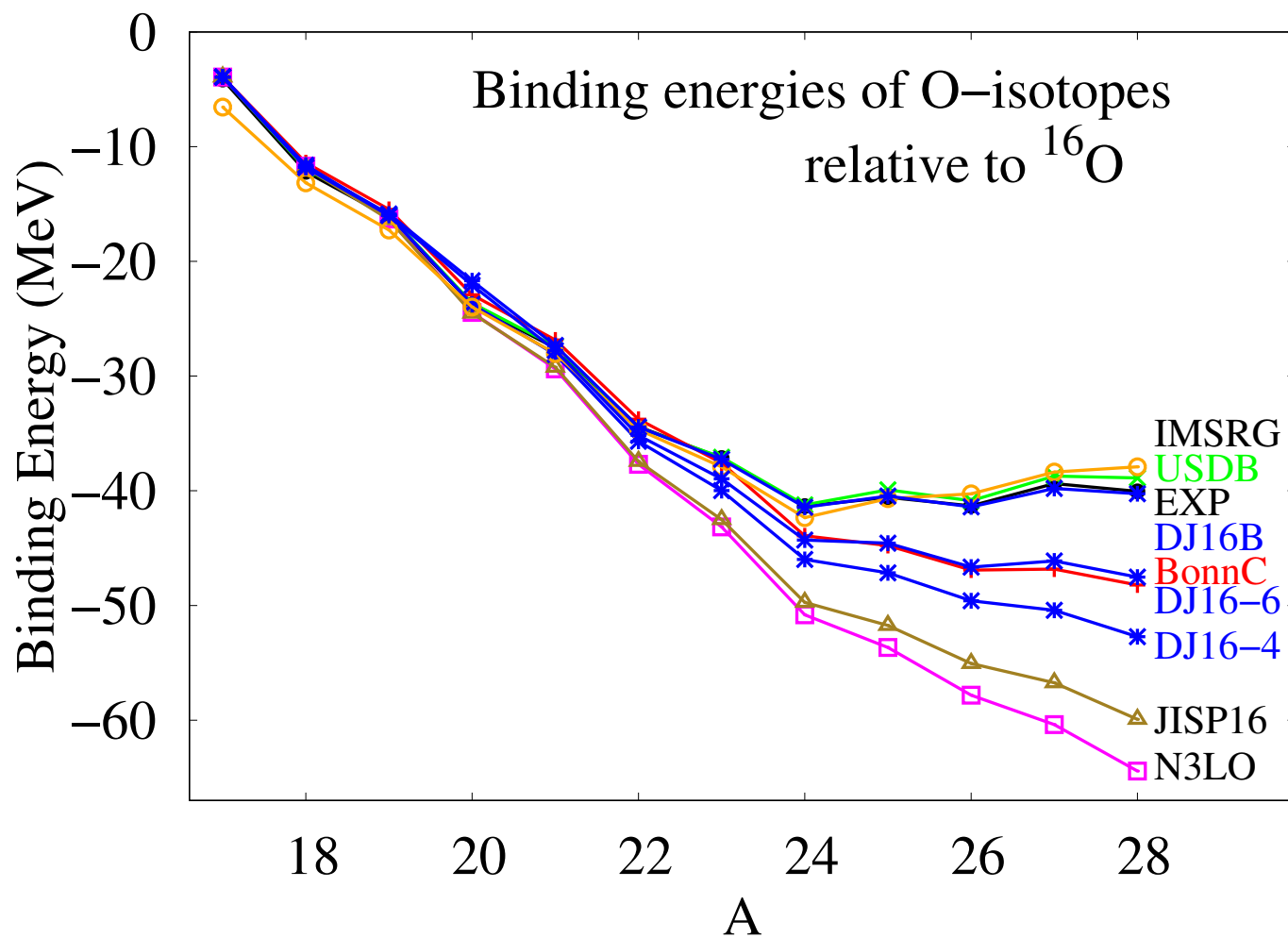
Dikmen, Lisetskiy, Barrett, Maris, Shirokov, Vary, *PRC91*, 064301 (2015)

Vary, Basili, Du, Lockner, Maris, Pal, Sarker, *PRC98*, 065502 (2018)

Smirnova, Barrett, Kim, Shin, Shirokov, Dikmen, Maris, Vary, *PRC100*, 054329 (2019)

See Nadezda Smirnova's talk on Thursday at 12 noon

# Binding energies of O-isotopes

$$\text{rms}(\text{DJ16-6}) \approx 3671 \text{ keV}; \quad \text{rms}(\text{DJ16B}) \approx 235 \text{ keV}; \quad \text{rms}(\text{USDB}) \approx 467 \text{ keV}$$




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

See talk by Peng Yin tomorrow at 10am

## 1. *Ab initio* structure calculation

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

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



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

## 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.* (in press); and in preparation

# d+<sup>208</sup>Pb scattering below Coulomb barrier

## tBF with no adjustable parameters

Solve EOM for CM motion in external field:

$V_I(t)$  = time-dependent electric dipole field

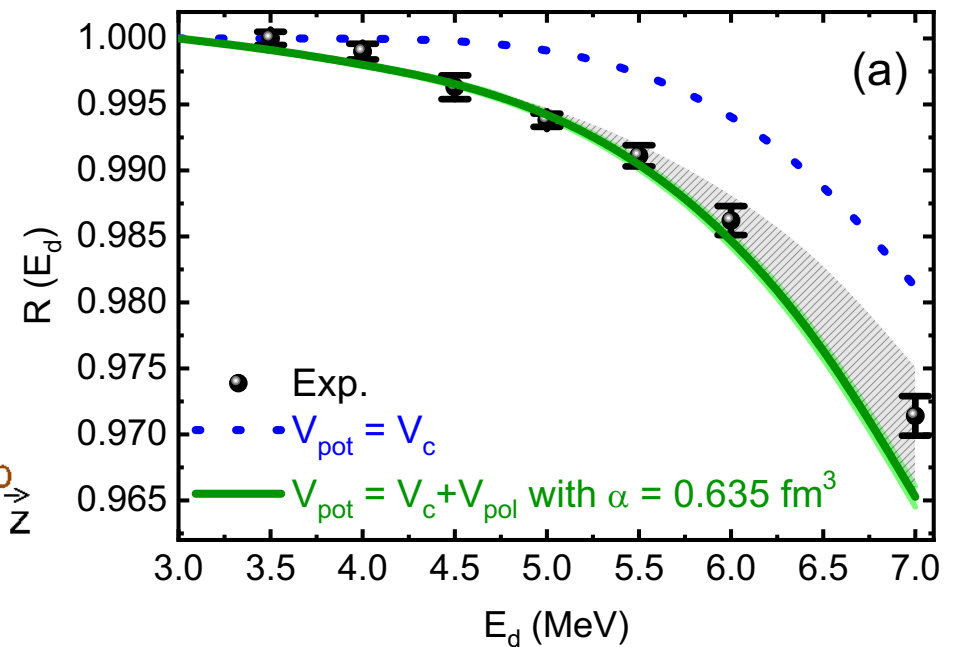
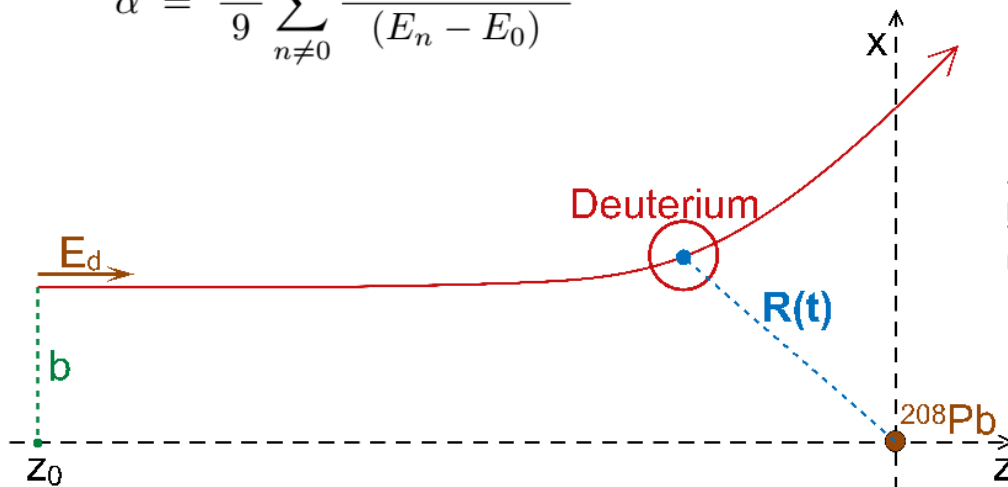
$$V_{\text{pot}} = V_c + V_{\text{pol}}$$

acting on np relative coordinates

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

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

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



- Scattering states of  $np$  system: LENPIC N4LO in 3DHO basis with large  $N_{\text{max}}$
- 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

## **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

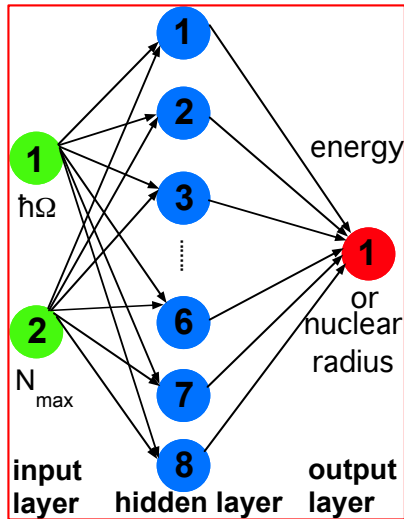
# Deep Learning for Nuclear Binding Energy and Radius

## Scientific Achievement

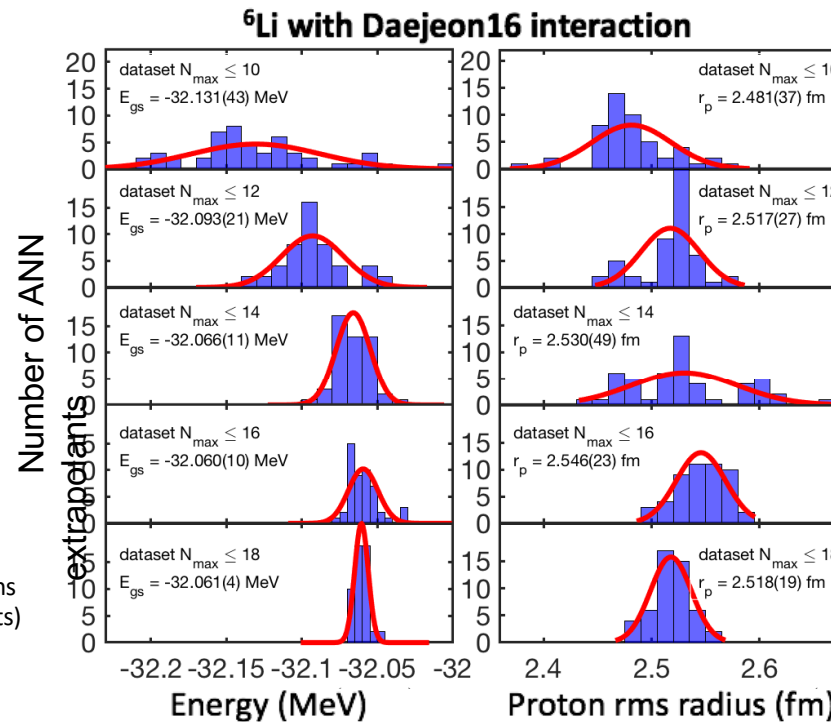
- Developed artificial neural networks (ANNs) for extending the application range of the *ab initio* No-Core Shell Model (NCSM)
- Demonstrated predictive power of ANNs for converged solutions of weakly converging simulations of the nuclear radius
- Provided a new paradigm for matching deep learning with 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  ${}^6\text{Li}$  ground state energy and rms radius from modest basis spaces ( $N_{\text{max}}$  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

# 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]

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

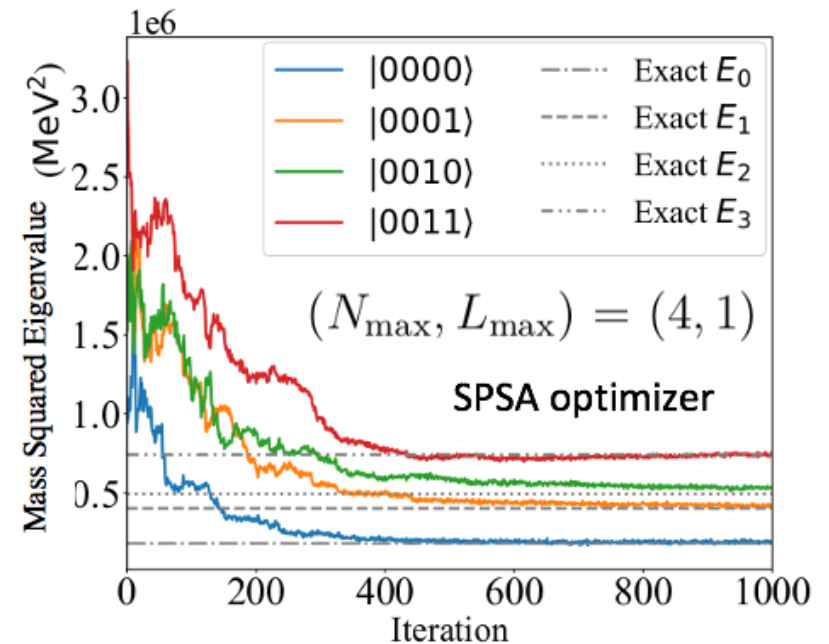
- Basis representation (BLFQ) is key to represent the Hamiltonian on qubits
- Small-size Hamiltonians (4-by-4 and 16-by-16) are used [Seeley, 1208.5986]
- Direct encoding and compact encoding are compared [Kreshchuk, 2002.04016]
- With evolved states: decay constants, PDFs, transition amplitudes, . .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

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

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

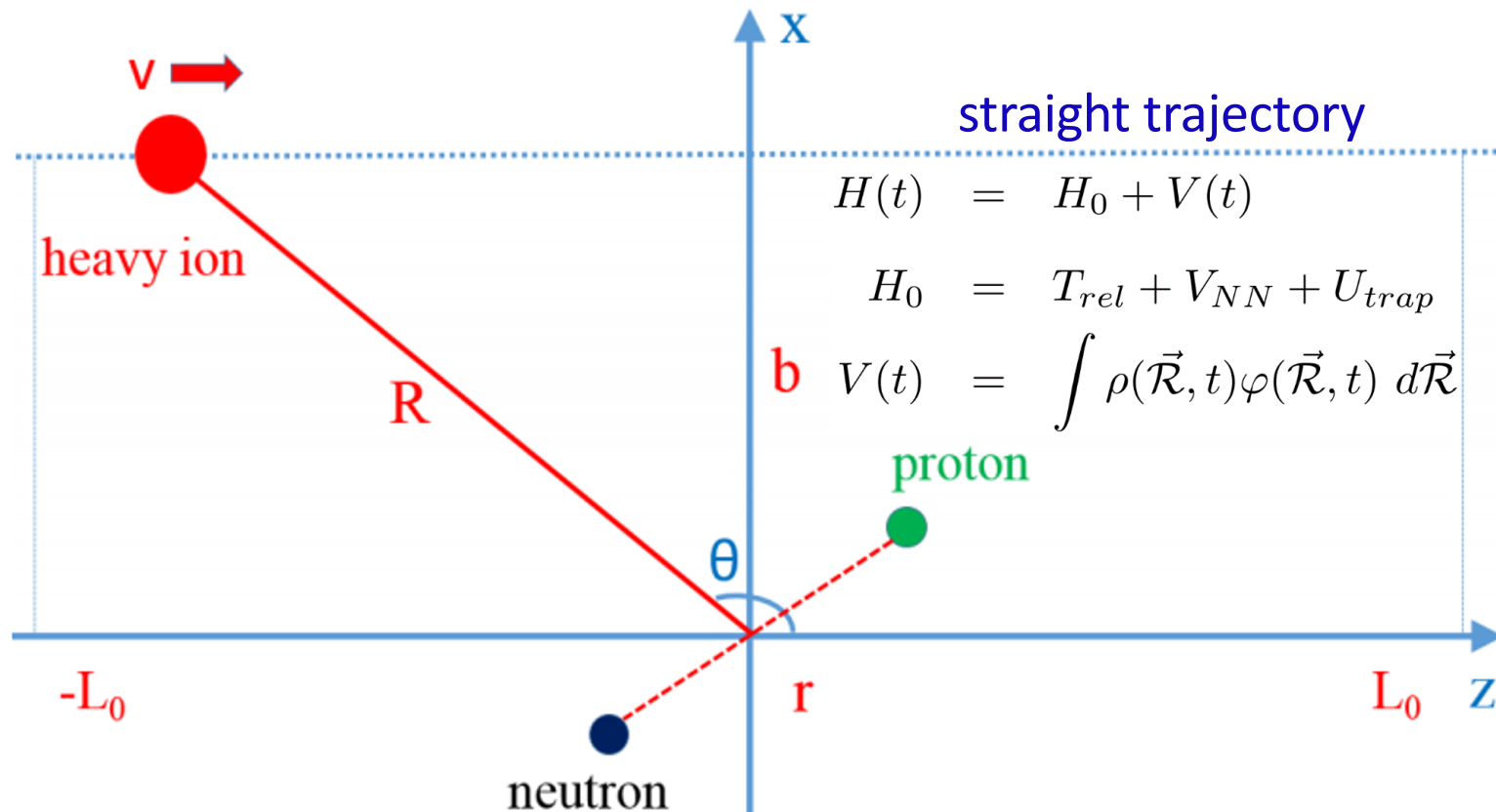
Fewer qubits, greater circuit depth (4-by-4 case):

$$H_{\text{compact}} = 1134731 \text{ II} - 566245 \text{ IZ} \\ + 4831 \text{ XI} + 20598 \text{ XZ}$$



# tBF on Quantum Computers

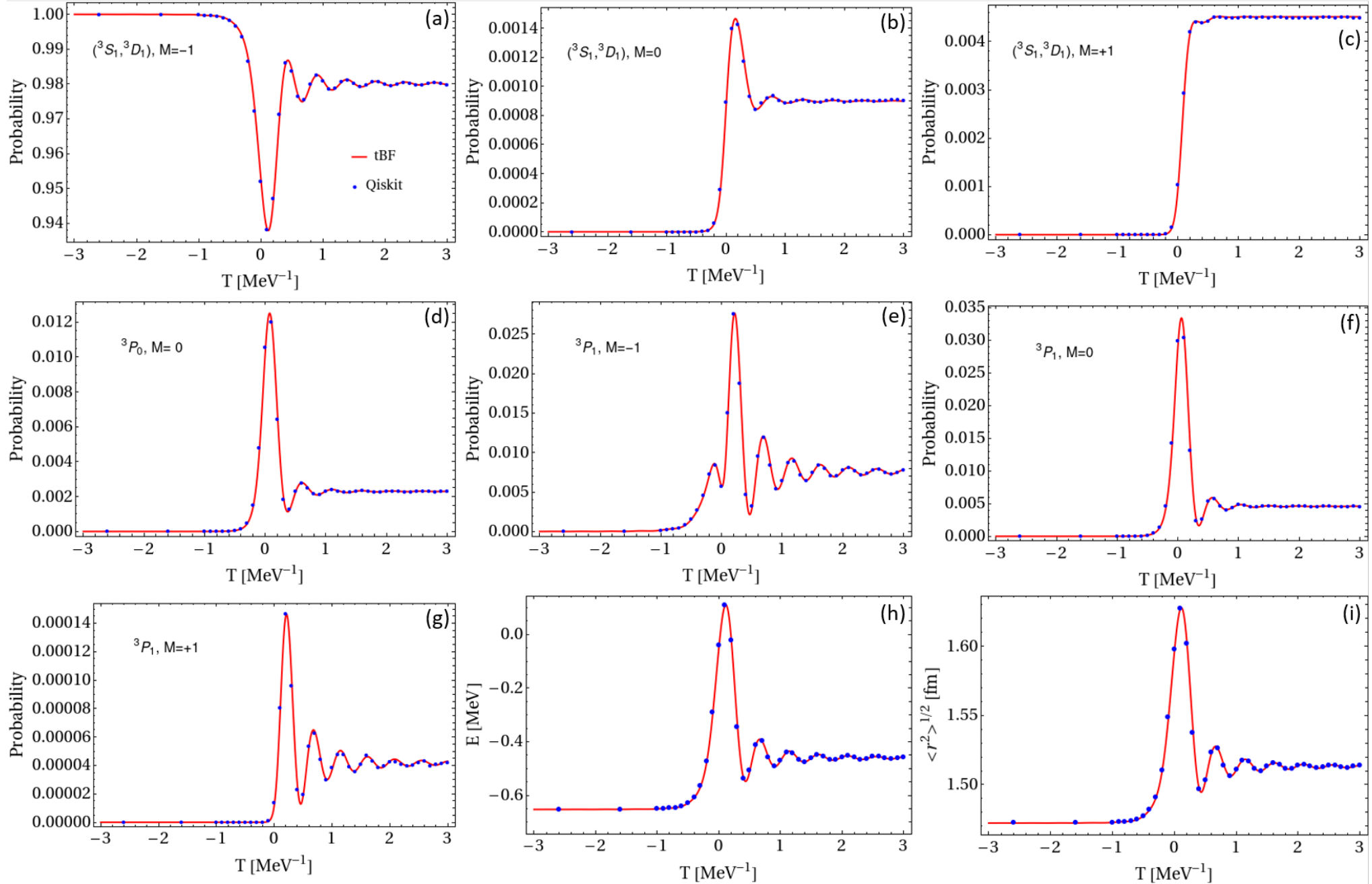
Demonstration case: Coulomb excitation of deuterium by peripheral scattering on a heavy ion



- $H_0$ : Target (deuteron in trap) Hamiltonian
- $\varphi$ : Coulomb field from heavy ion ( $U^{92+}$ ) sensed by target
- $\rho$ : 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





Many outstanding nuclear physics  
puzzles and discoveries remain

Spin structure of the proton

Exotic systems including glueballs

Clustering phenomena

Origin of the successful nuclear shell model

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