

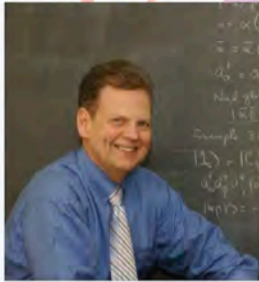
Big problems, Big computers and a Big man: Towards ab initio hadron physics with basis light-front quantization

Yang Li

University of Science and Technology of China

Nuclear Theory in the Supercomputing Era
Institute of Modern Physics & Zoom
June 5, 2023





“For distinguished contributions to our understanding of nuclear and hadronic structure, creating new computational frameworks for the many-body problem, and for fostering international collaboration in science.”

Citation for his fellowship of American Association for the Advancement of Science (2021)

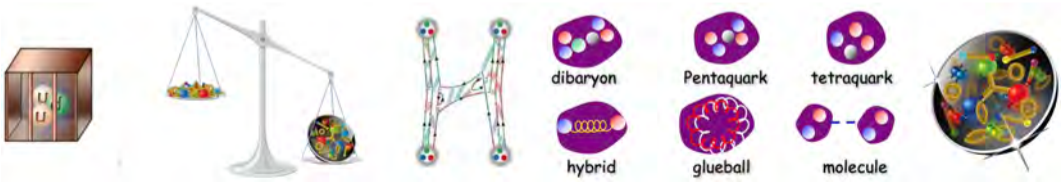
My first problem from Prof. Vary: solve for the structure of the proton



Disclosure: I was not able to solve the problem -- but I still got my Ph.D. at the mercy of Prof. Vary

Big questions with hadron structures

- Why is there no free quark or gluon observed in nature?
- Why is the proton much heavier than its constituent quarks?
- What is the origin of the nuclear force?
- What are the structures of the exotic hadrons?
- What are the distributions of quarks and gluons inside the hadrons?



A brief (and biased) history of hadron structures

- Proton magnetic moment (1930s)
- Elastic scattering of proton (1950s)
- Quark model (early 1960s)
- Chiral symmetry breaking (1960s)
- Deep inelastic scattering (late 1960s)
- Quantum chromodynamics (1970s)



Nobel prize 1943



Nobel prize 1951



Nobel prize 1969



Nobel prize 1990



Nobel prizes 1999 & 2004



Nobel prize 2008

BLFQ (June 5, 2023)

50 Years of Quantum Chromodynamics

Franz Gross^{a,1,2}, Eberhard Klempt^{b,3},

Stanley J. Brodsky^{c,4}, Andrzej J. Buras^{c,5}, Volker D. Burkert^{c,1}, Gudrun Heinrich^{c,6}, Karl Jakobs^{c,7}, Curtis A. Meyer^{c,8}, Kostas Orginos^{c,1,2}, Michael Strickland^{c,9}, Johanna Stachel^{c,10}, Giulia Zanderighi^{c,11,12},

5.4 Light-front quantization

James Vary, Yang Li, Chandan Mondal
and Xingbo Zhao

In this section, we discuss non-perturbative light-front Hamiltonian quantization methods. We primarily focus on introducing the Hamiltonians for QED and QCD derived in the light-cone gauge (for extensive reviews, see Refs [792, 908]). We introduce methods of solution and results for mesons and baryons. We focus on the Discretized Light Cone Quantization (DLCQ) and Basis Light Front Quantization (BLFQ) methods due to their ability to include gluons and sea quarks dynamically.

Light-front quantization is the natural language for

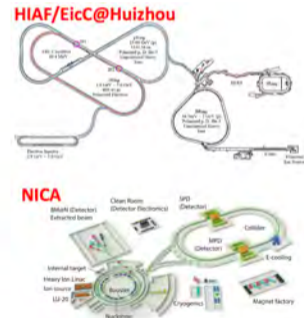
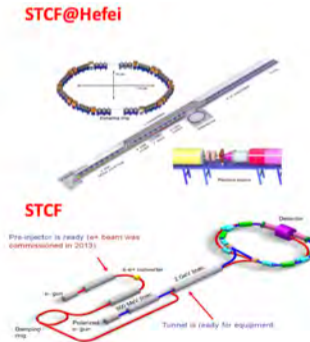
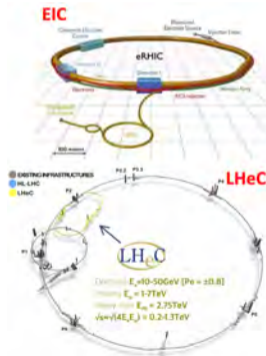
$$H = \sum_i \frac{p_i^{+2} + m_i^2}{x_i} + H_{int} + \lambda_{CM} H_{CM}. \quad (5.4.2)$$

Here, the sum is over all partons and m_i is the mass of the i^{th} parton. The role of the Lagrange multiplier term ensures factorization of the state vector's transverse component into an internal, boost invariant, component times a center of mass (CM) component [911].

We note that this eigenvalue problem applies to systems with arbitrary baryon number so that, for example, it applies to atomic nuclei as well. An eigenstate of a system can be written in terms of a Fock-space expansion over sectors with N -partons as

$$|P, A\rangle = \sum_N \sum_{\lambda_1, \dots, \lambda_N} \int \frac{\prod_{i=1}^N dx_i dp_i^\perp}{[2(2\pi)^N]^2 \sqrt{x_1 x_N}} \delta(1 - \sum_{i=1}^N x_i)$$

- Electron-ion colliders: eRHIC, EicC, LHeC [AbdulKhalek:2021gbh, Anderle:2021wcy, LHeC:2020van]
- Electron-positron colliders: superKEKB, Super τ -charm facility (STCF) [Peng:2020orp]
- Heavy ion colliders: NICA, HIAF, FAIR



Wilson's idea: put QCD into big computers



AB INITIO QUANTUM CHEMISTRY:
A SOURCE OF IDEAS FOR LATTICE GAUGE THEORISTS

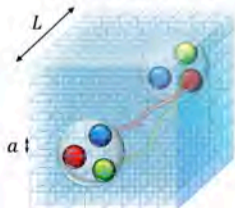
Ken Wilson, 1989
cf. Ken Wilson, 2005

Kenneth G. WILSON

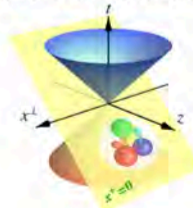
The Ohio State University, Department of Physics, 174 W. 18th Avenue, Columbus, OH 43210 USA

Ab initio quantum chemistry is an emerging computational area that is fifty years ahead of lattice gauge theory, a principal competitor for supercomputer time, and a rich source of new ideas and new approaches to the computation of many fermion systems. An overview of the history, current prospects and future frontiers of quantum chemistry is given, with special emphasis on lessons for lattice gauge theory. Particular reference is given to the role of Gaussian basis functions (in place of grids) and analytic (as opposed to Monte Carlo) methods. The main recommendation to lattice gauge theorists is for greater emphasis on infinite momentum frame studies, using Gaussian basis functions.

Lattice gauge theory



Light-front Hamiltonian theory



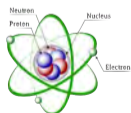
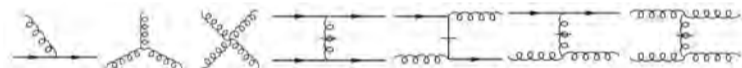
LFQCD as a strong-coupling relativistic quantum many-body problem

$$H_{\text{LFQCD}} = \sum_i \frac{\vec{p}_{i\perp}^2 + m_i^2}{x_i} + U_i + \sum_{ij} V_{ij}^{(\text{QCD})} - \delta_{ij} U_i$$

- Exponential wall: $\dim \mathcal{H} = N^{dN}$
- Moore's law, Quantum advantage?
- Semi-classical first approximation

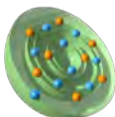
[Hornbostel:1988fb, Anand:2020gnn]

[Kreshchuk:2020dla]



Non-relativistic,
weakly coupling

Bohr Model 

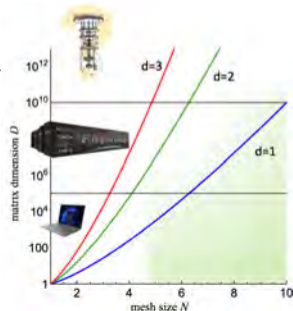


Non-relativistic,
strongly coupling

Shell Model 



Relativistic,
strongly coupling



Jacob's ladder

Jacob's ladder in quantum chemistry



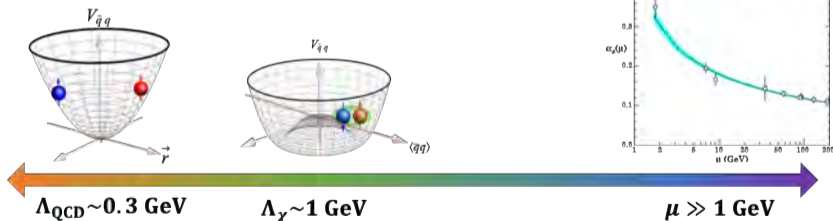
$$\left(\frac{\vec{k}_\perp^2 + m_q^2}{x} + \frac{\vec{k}_\perp^2 + m_{\bar{q}}^2}{1-x} + U \right) \psi(x, \vec{k}_\perp) = M^2 \psi(x, \vec{k}_\perp)$$

factorization ansatz $\Downarrow \psi = \varphi(\vec{\zeta}_\perp) \chi(x)$

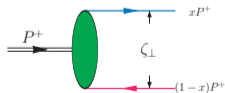
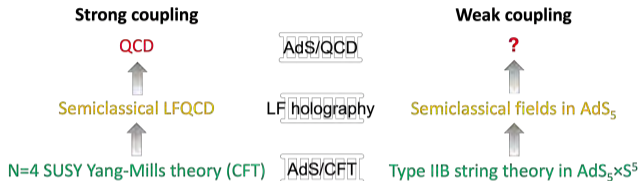
$$\left[-\nabla_{\zeta_\perp}^2 + U_\perp(\vec{\zeta}_\perp) \right] \varphi(\vec{\zeta}_\perp) = M_\perp^2 \varphi(\vec{\zeta}_\perp), \quad \left[\frac{m_q^2}{x} + \frac{m_{\bar{q}}^2}{1-x} + U_\parallel(\tilde{z}) \right] \chi(x) = M_\parallel^2 \chi(x)$$

where $\vec{\zeta}_\perp = \sqrt{x(1-x)} \vec{r}_\perp$.

$U_{\text{eff}}(\zeta_\perp)$



Light-front holography provides a unique correspondence between semiclassical LFQCD and semiclassical fields in 5D anti-de Sitter space



semiclassical LFQCD

$$\zeta_{\perp} = \sqrt{x(1-x)}r_{\perp}$$

LF amplitude

confining potential

$$L^2 - (J - 2)^2$$

form factors

\leftrightarrow

semiclassical field theory in AdS

\leftrightarrow

fifth coordinate z ,

\leftrightarrow

string amplitude

\leftrightarrow

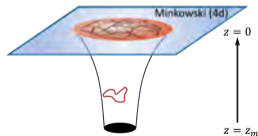
dilation field Φ

\leftrightarrow

$$(\mu R)^2$$

\leftrightarrow

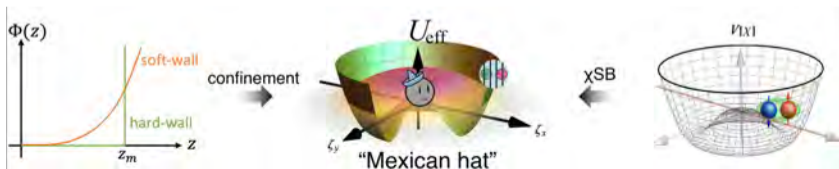
form factors



Confinement & chiral symmetry breaking in holographic QCD

$$S = - \int d^5x \sqrt{-g} e^{-\Phi(z)} \text{Tr} \left\{ |DX|^2 - V[X] + \frac{1}{4g_5^2} F^2 \right\},$$

- Confinement: breaking of the conformal symmetry at the IR ($z \rightarrow \infty$) [Erich:2005qh]
 - Dilaton field $\Phi(z)$
 - Soft-wall model reproduces Regge trajectory: $\Phi(z \rightarrow \infty) \sim z^2 \Rightarrow U(z) \sim z^2$ [Karch:2006pv]
- Chiral symmetry breaking: Higgs condensate $\langle X \rangle = \frac{1}{2} \chi(z)$ [Gherghetta:2009ac]
 - Scalar field X is dual to $\bar{q}q$
 - Higgs potential: $V[X] = -m_X^2 |X|^2 + \kappa |X|^4$, $m_X^2 = -3$ [Kapusta:2010mf]
 - Condensate at CFT boundary ($z \rightarrow 0$): $\chi(z) \sim m_q z + \Sigma z^3 \Rightarrow U(z) \sim -z^4$ [Klebanov:1999tb]
- χ SB & confinement dictate the UV & IR behaviors of $U(z)$, respectively [Li:2022ytx]



Chiral symmetry breaking on the light front

χ SB is encoded in the hadronic LFWFs

[Casher:1974xd, Burkardt:1996pa, Wu:2003vn, Beane:2013oia, Beane:2015ufo]

- Light-front vacuum & zero modes: $Q_5|0\rangle_{LF} = 0$

[Brodsky:2010xf]

- The most general covariant structure of pion LFWFs including zero modes

[Carbonell:1998rj]

$$\psi_{s\bar{s}/P}(x, \vec{k}_\perp) = \bar{u}_s(p_1) \left[\gamma_5 \phi_1(x, k_\perp) + \hat{f}_x \frac{\gamma_5 \psi}{\omega \cdot p} \phi_2(x, k_\perp) \right] v_{\bar{s}}(p_2),$$

- Partially conserved axial-vector current (PCAC) leads to a light-front chiral sum rule:

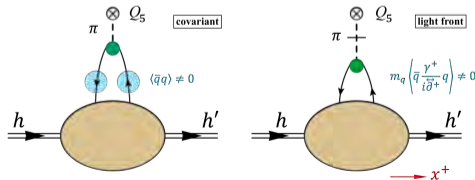
[Li:2022ytx]

$$\int \frac{dx}{2\sqrt{x(1-x)}} \int \frac{d^2k_\perp}{(2\pi)^3} \frac{k_\perp^2}{x(1-x)} \psi_{\uparrow\downarrow-\downarrow\uparrow/P}^{(0)}(x, \vec{k}_\perp) = 0 \quad \xrightarrow{\text{LFH}} \quad f_P \nabla_\perp^2 \varphi_P(\zeta_\perp = 0) = 0$$

- Gell-Mann-Oakes-Renner relation: $f_P^{(0)2} M_P^2 = 2m_q g_P^{(0)} + O(m_q^2)$, where $g_P = \langle 0 | j_5 | P(p) \rangle$

- Similar idea in DSE/BSE: AvWTI leads to $f_\pi E_\pi(k, 0) = B_q(k^2), \dots$

[Maris:1997hd]



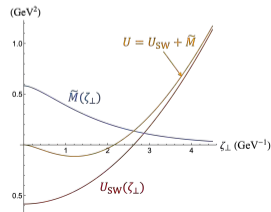
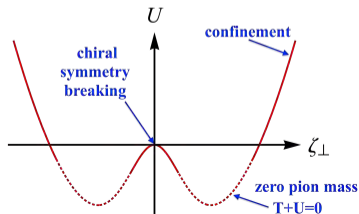
$$\left[-\nabla_{\perp}^2 + U(\zeta_{\perp}) \right] \varphi_h(\zeta_{\perp}) = M_h^2 \varphi_h(\zeta_{\perp}), \quad \nabla_{\perp}^2 \varphi_P(\zeta_{\perp} = 0) = 0, \quad U(\zeta_{\perp}) \rightarrow \begin{cases} \zeta_{\perp}^2 & \zeta_{\perp} \rightarrow \infty \\ -\zeta_{\perp}^4 & \zeta_{\perp} \rightarrow 0 \end{cases}$$

$$\left[\frac{m_q^2}{x} + \frac{m_{\bar{q}}^2}{1-x} + U_{\parallel} \right] \chi(x) = M_{\parallel}^2 \chi(x),$$

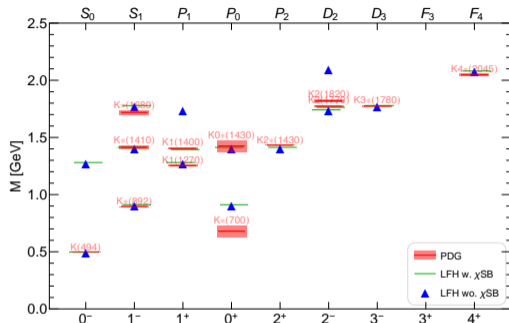
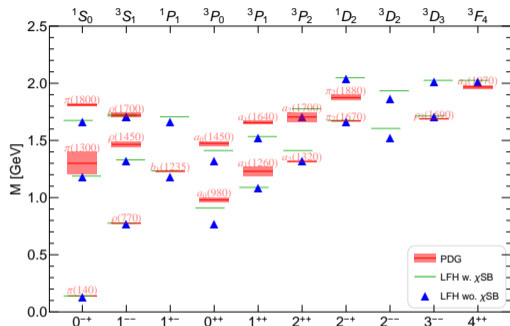
The pion: $f_{\pi} \neq 0, M_{\pi} = 0, \Rightarrow U(\zeta_{\perp} = 0) = 0$ (cf. $U_{\text{Higgs}} \sim -\zeta_{\perp}^4 \rightarrow 0$),

- Transverse: Mexican hat potential [Li:2022ytx]
- Longitudinal: Li-Maris-Zhao-Vary potential $U_{\parallel} = -\sigma^2 \partial_x (x(1-x)\partial_x)$ similar to 't Hooft model, Gell-Mann Oakes Renner relation

[Li:2021jqb, cf. deTeramond:2021yyi, Ahmady:2021lsh, Ahmady:2021yzh, Lyubovitskij:2022rod, Ahmady:2022dfv]



Spectra of unflavored light mesons



- Semiclassical LFQCD with confinement and with/without chiral symmetry breaking

[Brodsky:2014yha, Li:2021jqb]

- State identification with relativistic quantum numbers, $n, m, l, J, S \rightarrow J^{PC}(N^{2S+1}L_J)$

- $C = (-1)^{m+l+S}, (-1)^{JP} = (-1)^{m+S+1}$

Pion electromagnetic form factor & parton distribution function

- Holographic current: Veneziano amplitude

[Grigoryan:2007wn, deTeramond:2018ecg, Liu:2019vsn]

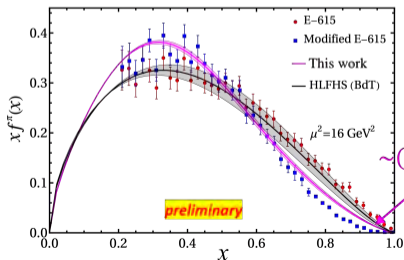
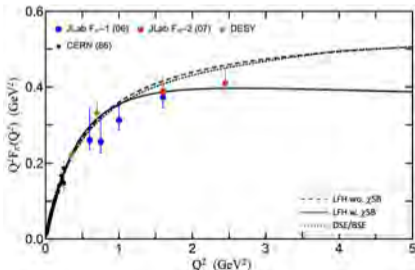
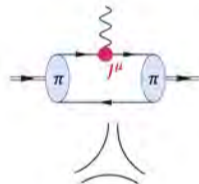
- χ SB incorporates high-twist contributions: Brodsky-Farrar counting rule ($\tau = N$)

[Li:2022ytX]

$$F_{\pi}(q^2) = N \left\{ \underbrace{F_{\tau=2}(q^2)}_{[q\bar{q}]} + \underbrace{F_{\tau=3}(q^2)}_{[q\bar{q}g]} + c_1 \underbrace{F_{\tau=4}(q^2)}_{[q\bar{q}q\bar{q}]} + \dots \right\}$$

- Generalized parton distribution (GPD)

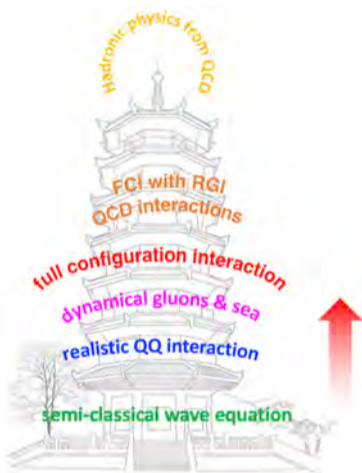
$$F_{\pi}(q^2) = \int dx H_{\pi}(x, t = q^2), \quad f_v(x) = H_{\pi}(x, t = 0)$$



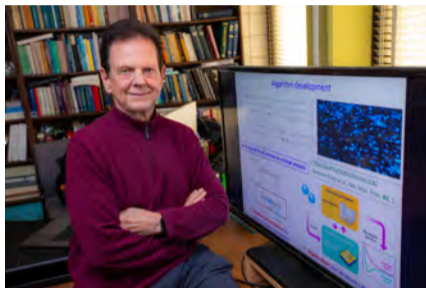
Global analysis:
 $\sim (1-x)^{1.0 \sim 1.3}$

[Barry:2021osv]

Jacob's tower



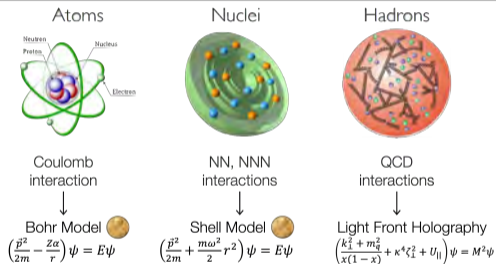
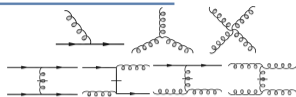
Big computers to solve big problems



Yang, we are not much smarter than those big names in the 70s, but we certainly have much bigger computers, and they get bigger.

Light-front QCD in
light cone gauge $A^+ = 0$

$$H_{\text{LFQCD}} = \sum_i \frac{\vec{p}_{i\perp}^2 + m_i^2}{x_i} + \sum_{ij} V_{ij}^{(\text{QCD})}$$

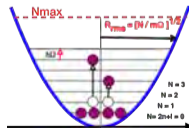


It is important to preserve all kinematical symmetries under the truncation

- Discretized momentum basis (DLCQ) → Lagrange mesh (continuum method)

[Hornbostel:1988fb, Trittman:1997xz, Lamm:2013oga, Li:2015iaw]

- Basis light-front quantization (BLFQ) [Vary:2009gt]



[Review: Barrett:2013nh (NCSM)]

BLFQ (June 5, 2023)

Basis light-front quantization

- Configuration interaction:

[Vary:2009gt]

$$H|\psi\rangle = M^2|\psi\rangle \quad \Rightarrow \quad \sum_j H_{ij}c_j = M^2c_i$$

where, $H_{ij} = \langle\phi_i|H|\phi_j\rangle$, $c_i = \langle\phi_i|\psi\rangle$.

- Single-particle basis $\{|\phi_i\rangle\}$ is chosen to **preserve all kinematical symmetries** of QCD
 - 3 Boosts + 1 rotation:

$$\phi_{nml}(\vec{x}_\perp, x^-) = \mathcal{N} e^{\frac{i\pi l x^-}{L} + im\theta_\perp - \frac{\rho^2}{2}} \rho^{|m|} L_n^{|m|}(\rho), \quad (\rho = \Omega\sqrt{l/K}x_\perp)$$

- Longitudinal direction: discretized momentum basis, Jacobi polynomials on a k -simplex
[Chabysheva:2013oka, Li:2017mlw]
 - Other symmetries of QCD
- Consistent with holographic LFQCD
- Large sparse matrix eigenvalue problem: suitable for modern HPC (& quantum computing?)

Finite basis truncations in BLFQ

- Energy cutoffs/regularization:

$$\sum_i [2n_i + |m_i| + 1] \leq N_{\max}, \quad \sum_i m_i + s_i = m_J, \quad \sum_i l_i = K.$$

- UV & IR regulators:

$$\Lambda_{\text{UV}} = \Omega \sqrt{N_{\max}}, \quad \Lambda_{\text{IR}} = \Omega / \sqrt{N_{\max}}$$

- Truncation on the many-body basis:

- Fock sector truncation
- N_{\max} -truncation, K -truncation
- Coupled cluster/coherent basis
- DMRG, matrix product states, tensor network, ...

[Hiller:2016itl, More:2014rna]

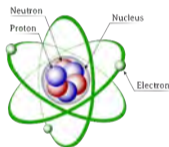
- Variational theorem
- Continuum limit (need a proof):

$$N_{\max} \rightarrow \infty, \quad K \rightarrow \infty, \quad A \rightarrow \infty$$

Semi-classical first approximation: first order

$$H = \sum_i \frac{p_{i\perp}^2 + m_i^2}{x_i} + U_i^{(0)} + \sum_{ij} \alpha_s U_{ij}^{(1)} + \sum_{ij} V_{ij} - U_{ij}$$

Atoms



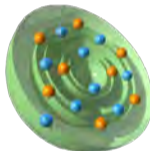
Bohr Model 

$$\left(\frac{\vec{p}^2}{2m} - \frac{Z\alpha}{r} \right) \psi = E\psi$$



L-S coupling, ...

Nuclei



Shell Model 

$$\left(\frac{\vec{p}^2}{2m} + \frac{m\omega^2}{2} r^2 \right) \psi = E\psi$$



L-S coupling, ...

Hadrons



Light Front Holography

$$\left(\frac{\vec{k}_\perp^2}{x(1-x)} + \kappa^4 \zeta_\perp^2 + U_{||} \right) \psi = M^2 \psi$$



One-gluon exchange

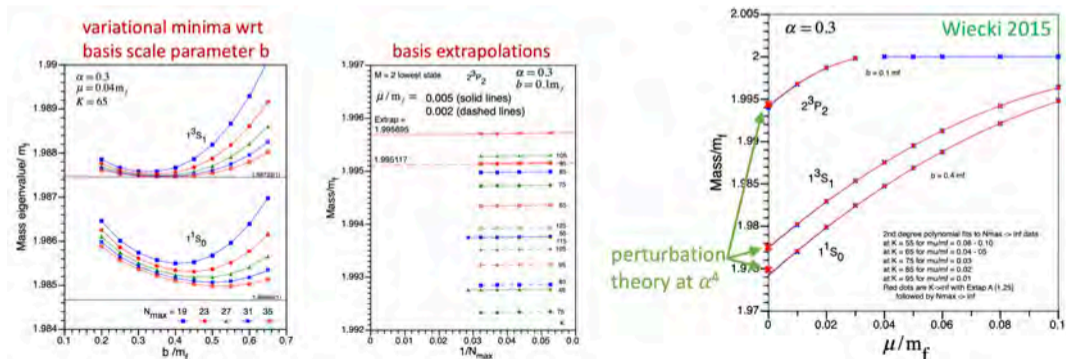
- Bloch-Wilson interaction: perturbative solution to the OSL effective Hamiltonian [Krautgartner:1991xz]

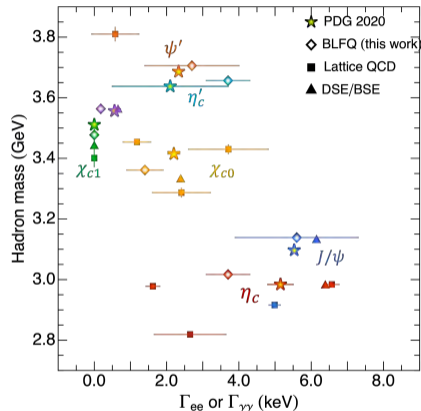
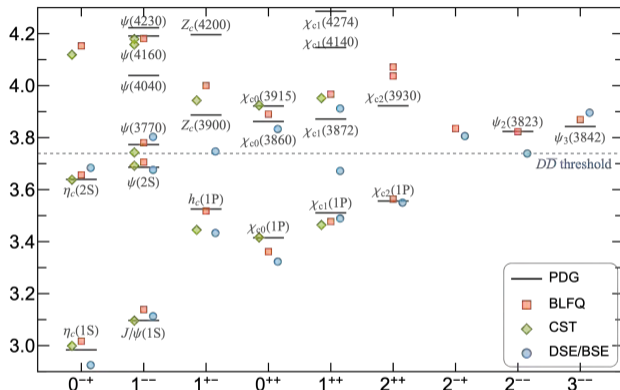
$$\alpha_s U^{(1)} = \frac{C_F 4\pi\alpha_s(Q^2)}{Q^2} \bar{u}_{s'}(k') \gamma_\mu u_s(k) \bar{v}_{\bar{s}}(\bar{k}) \gamma^\mu v_{\bar{s}'}(\bar{k}')$$

- Benchmark (LFQED): striking agreement with perturbative QED results up to $O(\alpha^4)$:

$$H = T + H_{\text{Col}} + H_{\text{Dar}} + H_{\text{rel}} + H_{\text{LS}} + H_{\text{SS}}$$

[cf. Lamm:2016djr]





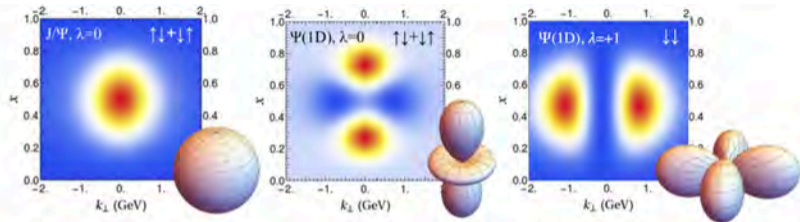
■ Two free parameters (m_c, κ), rms deviation: 30 MeV

■ Good agreement with the PDG data for both the masses and the widths

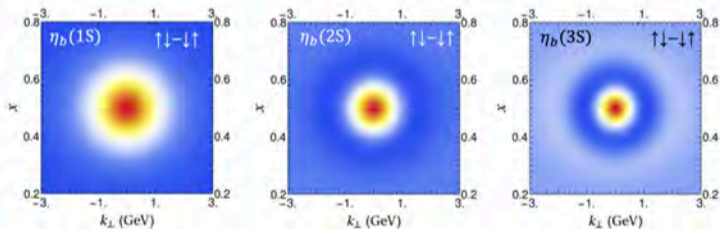
[Gross:2022hyw]

Quarkonium light-front wave functions

angular
excitation
S



radial
excitation
S

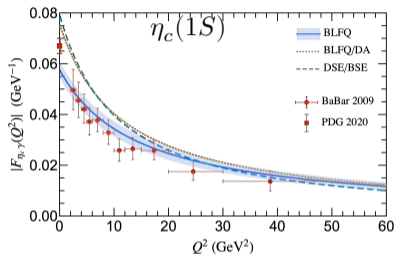


[LFWFs published on Mendeley Data, doi: 10.17632/cjs4ykv8cv.2]

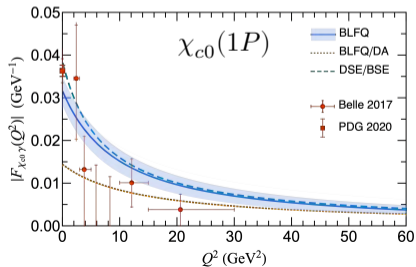
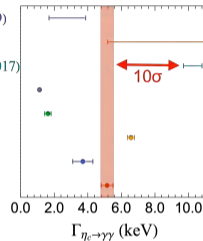
Parameter-free predictions for the diphoton transition form factors

Very challenging for NRQCD, Lattice QCD and quark models

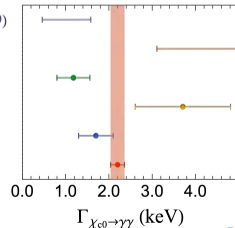
[Feng:2015uha, Feng:2017hlu, Meng:2021ecs, Colquhoun:2023zbc, Christ:2022rho]



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



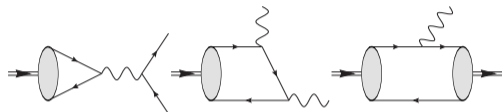
NRQM/LF (Babiarz 2019)
NRQM (Babiarz 2019)
Lattice (Chen 2020)
Lattice (Zou 2021)
BLFQ (this work)
PDG 2020



All radiative transitions

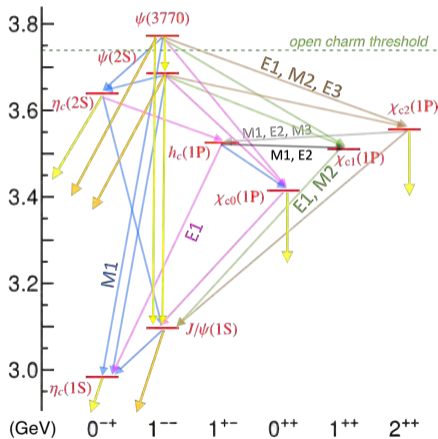
Leptonic and radiative transitions probe the fundamental structure of the hadrons:

[Review: Barnes & Yuan, Int. J. Mod. Phys. A 2009]

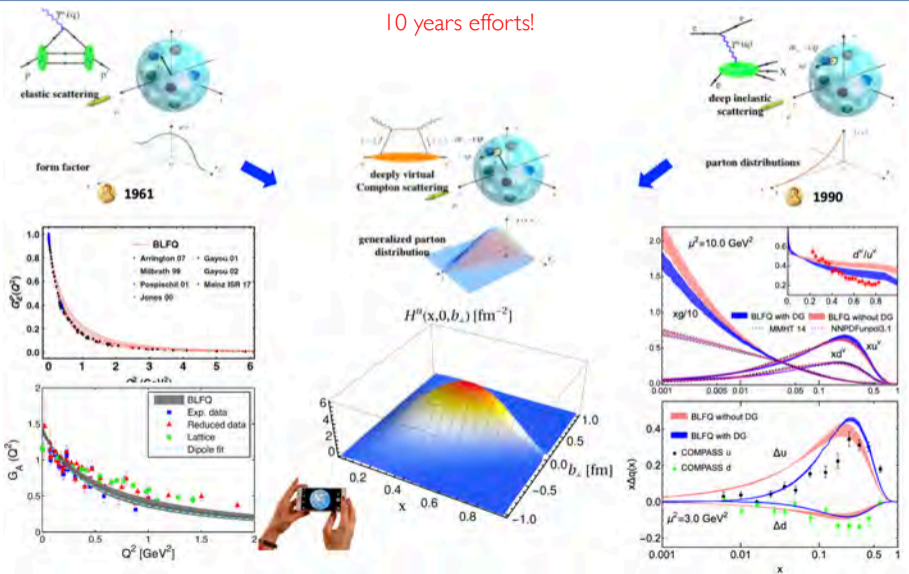


decay width (keV)		Γ_{ee}	$\Gamma_{\gamma\gamma}$		
η_c	PDG	-	5.15(35)		
	BLFQ	-	3.7(6)	$\Gamma_{\eta_c\gamma}$	
J/ψ	PDG	5.53(10)	-	1.6(4)	
	BLFQ	5.7(1.9)	-	2.6(1)	$\Gamma_{J/\psi\gamma}$
χ_{c0}	PDG	-	2.1(1.6)	-	$15(1) \times 10^3$
	BLFQ	-	1.9(4)	-	in progress
χ_{c1}	PDG	-	-	-	288(16)
	BLFQ	-	-	-	in progress
\vdots					

[YL, PRD '17; Li, PRD '18; Wang, in progress]



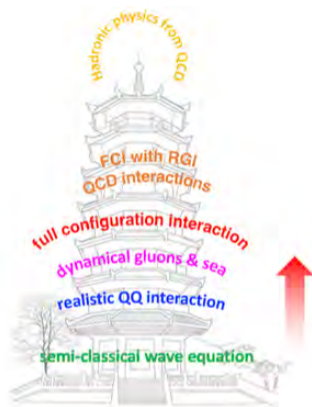
10 years efforts!



- Semi-classical LF wave equations: [Li:2021jqb, Li:2022izo, Li:2022ytx, cf. deTeramond:2021yyi, Ahmady:2021lsh, Ahmady:2021yzh, Lyubovitskij:2022rod, Ahmady:2022dfv]
- Realistic QQ interaction:
 - QED: [Honkanen:2010rc, Zhao:2014xaa, Wiecki:2014ola, Hu:2020arv, Nair:2022evk, Nair:2023lir]
 - heavy flavors [Li:2015zda, Li:2017mlw, Leitao:2017esb, Li:2018uif, Adhikari:2018umb, Tang:2018myz, Lan:2019img, Tang:2019gvn, Tang:2020org, Li:2021ejv, Li:2021cwv, Shuryak:2021fsu, Shuryak:2021hng, Shuryak:2021mlh, Shuryak:2022thi, Shuryak:2022wtk]
 - light mesons [Jia:2018ary, Lan:2019vui, Lan:2019rba, Qian:2020utg, Mondal:2021czk, Adhikari:2021jrh, Li:2022mlg]
 - nucleons [Mondal:2019jdg, Xu:2021wwj, Liu:2022fvl, Hu:2022ctr, Peng:2022lte, Zhu:2023lst]
 - tetraquarks [Kuang:2022vdy]
- Dynamical gluons & sea: [Lan:2021wok, Xu:2022abw]
- Time-dependent problems (tBLFQ): [Zhao:2013cma, Zhao:2013jia, Chen:2017uuq, Li:2020uhl, Li:2023jeh]
- Hadronic physics on quantum computer: [Kreshchuk:2020kcz, Kreshchuk:2020aiq, Qian:2021jxp]

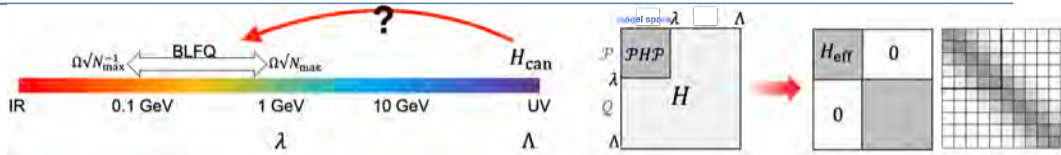


Jacob's tower



“更上一层楼” (“take it to the next level”)

Renormalization in non-perturbative Hamiltonian formalism



- Standard renormalization (Weinbergian renormalization):

$$H_R = \underbrace{H_{\text{can}}}_{\text{divergence}} + \underbrace{H_{\text{ct}}}_{\text{divergence}} = H_{\text{can}} + \sum_i c_i O_i$$

- Wilsonian renormalization: low-energy effective Hamiltonian with similarity renormalization group (SRG) transformations

[Glazek:1993rc, Wilson:1994fk, Glazek:2012qj]

$$H_s = \underbrace{U_s^{-1} H_\infty U_s}_{\text{divergence free}}$$

- Renormalized realistic QQ interactions: Ôkubo-Suzuki-Lee (OSL)

[Suzuki:1980yp]

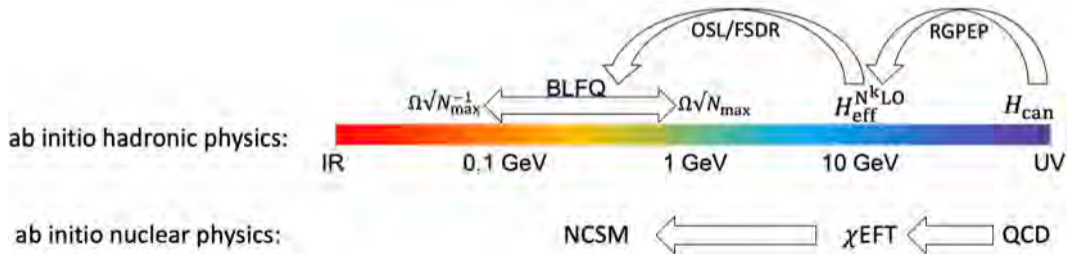
$$H_{\text{eff}} = \mathcal{P} X H_0 X^{-1} \mathcal{P}$$

- Fock sector dependent renormalization

[Karmanov:2008br, Li:2015iaw]

Towards ab initio LFGCD

- $H_\infty \rightarrow H_s$: generate a renormalized Hamiltonian H_s at some finite pQCD scale s with RGPEP
- $H_s \rightarrow H_{\text{eff}}^{(\Omega)}$: generate a low-energy few-body Hamiltonian $H_{\text{eff}}^{(\Omega)}$ at some hadron scale $\Omega\sqrt{N_{\text{max}}}$ with OSL
- Diagonalize $H_{\text{eff}}^{(\Omega)}$ with BLFQ



Summary

- Light-front Hamiltonian formalism is a natural framework to describe hadrons as relativistic quantum many-body problems
- Holographic LFQCD provides an adequate first approximation to QCD
- Basis light-front quantization provides an avenue to solving QCD from first principles

Thank you!

Happy birthday, Prof. James Vary



更上一层楼

Take it to the next level