Ab initio nuclear theory's symbiosis with relativistic quantum field theory

James P. Vary

Department of Physics and Astronomy Iowa State University Ames, USA

Nuclear Physics from Lattice QCD Institute for Nuclear Theory, UW, Seattle, QA May 24, 2016

"I worry that there is not enough research on approaches to solving QCD that could be complementary to Monte Carlo simulations, such as the lack of any comparable research built upon light-front QCD."

"…there needs to be more attention to research on light-front QCD as a complement to research on lattice gauge theory."

K.G. Wilson, "The Origins of Lattice Gauge Theory," Nuclear Physics B, Suppl., **140** (2005) p3

Barrett, Navrátil, Vary, *Ab initio no-core shell model*, PPNP69, 131 (2013)

Given a Hamiltonian operator

$$
\mathbf{\hat{H}} = \sum_{i < j} \frac{(\vec{p_i} - \vec{p_j})^2}{2 \, m \, A} + \sum_{i < j} V_{ij} + \sum_{i < j < k} V_{ijk} + \dots
$$

solve the eigenvalue problem for wavefunction of A nucleons

$$
\mathbf{\hat{H}}\Psi(r_1,\ldots,r_A) = \lambda \Psi(r_1,\ldots,r_A)
$$

- Expand eigenstates in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Diagonalize Hamiltonian matrix $H_{ij} = \langle \Phi_j | \hat{\mathbf{H}} | \Phi_i \rangle$
- No-Core CI: all A nucleons are treated the same
- Complete basis $→$ exact result
- In practice
	- truncate basis
	- study behavior of observables as function of truncation

Nuclei represent strongly interacting, self-bound, open systems with multiple scales – a computationally hard problem whose solution has potential impacts on other fields

Question: What controls convergence/uncertainties of observables?

Answer: Characteristic infrared (IR) and ultraviolet (UV) scales of the operators.

In a plane-wave basis:

- λ = lowest momentum scale can be zero (e.g. T_{rel}, r², B(EL), ...)
- Λ = highest momentum scale can be infinity (e.g. T_{rel} , hard-core V_{NN})

In a harmonic-oscillator basis with N_{max} truncation (Max total # oscillator quanta):

$$
\lambda \approx \sqrt{\hbar \Omega / N_{\text{max}}}
$$

$$
\Lambda \approx \sqrt{\hbar \Omega / N_{\text{max}}}
$$

What are examples of the other physically relevant scales in nuclear physics? Interaction scales (total binding, Fermi momentum, SRCs, one-pion exchange, . . .) Leading dissociation scale (halos, nucleon removal energy, . . .) Collective motion, clustering scales (Q, B(E2), giant modes, . . .)

Dirac's Forms of Relativistic Dynamics [Dirac, Rev.Mod.Phys. '49] Front form defines QCD on the light front (LF) $x^+ \triangleq t + z = 0$.

Nuclear interaction from chiral perturbation theory

- Strong interaction in principle calculable from QCD
- Use chiral perturbation theory to obtain effective A-body interaction from QCD Entem and Machleidt, PRC68, 041001 (2003)
	- controlled power series expansion in Q/Λ_χ with $\Lambda_\chi \sim 1$ GeV
	- natural hierarchy \bullet for many-body forces

 $V_{NNN} \gg V_{NNN} \gg V_{NNNN}$

- \bullet in principle no free parameters
	- in practice a few undetermined parameters
- renormalization necessary

Leading-order 3N forces in chiral EFT

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

Discretized Light Cone Quantization Pauli & Brodsky c1985

Basis Light Front Quantization*

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

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

Furthermore, f_{α} \rightarrow (\vec{x}) are arbitrary except for conditions: \rightarrow $\sqrt[*]{\vec{x}}$

Orthonormal:
$$
\int f_{\alpha}(\vec{x}) f_{\alpha}^{*}(\vec{x}) d^{3}x = \delta_{\alpha\alpha}
$$

\n**Complete:**
$$
\sum_{\alpha} f_{\alpha}(\vec{x}) f_{\alpha}^{*}(\vec{x}) = \delta^{3}(\vec{x} - \vec{x}')
$$

 \Rightarrow Wide range of choices for $f_a(\vec{x})$ and our <u>initial</u> choice is \rightarrow (\vec{x})

$$
f_{\alpha}(\vec{x}) = Ne^{ik^{+}x^{-}}\Psi_{n,m}(\rho,\varphi) = Ne^{ik^{+}x^{-}}f_{n,m}(\rho)\chi_{m}(\varphi)
$$

nu.e. vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de.
P. Sternberg, E.G. Ng and C. Yang, PRC 81, 035205 (2010). ArXiv:0905:1411 *J.P. Vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de Teramond,

Set of Transverse 2D HO Modes for n=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 Highlights

BLFQ introduced: J. P. Vary, H. Honkanen, Jun Li, P. Maris, S. J. Brodsky, A. Harindranath, G. F. de Teramond, P. Sternberg, E. G. Ng, C. Yang, Phys. Rev. C 81, 035205 (2010); arXiv: 0905.1411

Successfully applied to QED test cases – electron in a trap: H. Honkanen, P. Maris, J.P. Vary, S.J. Brodsky, Phys. Rev. Lett. 106, 061603 (2011); arXiv: 1008.0068

Introduced non-peturbative scattering in time-dependent BLFQ (tBLFQ): X. Zhao, A. Ilderton, P. Maris and J. P. Vary, Phys. Rev. D 88, 065014 (2013); arXiv: 1303.3237

tBLFQ successfully applied with time and space-dependent external fields: X. Zhao, A. Ilderton, P. Maris and J. P. Vary, Phys. Letts. B 726, 856 (2013); arXiv: 1309.5338

Improvements to BLFQ for QED test cases: trap independence, renormalization, . . . X. Zhao, H. Honkanen, P. Maris, J.P. Vary, S.J. Brodsky, Phys. Letts. B 737, 65 (2014); arXiv:1402.4195

Positronium at strong coupling: P. Wiecki, Y. Li, X. Zhao, P. Maris and J.P. Vary, Phys. Rev. D 91, 105009 (2015); arXiv 1404.6234

FFs and GPDs evaluated for positronium at strong coupling: L. Adhikari, Y. Li, X. Zhao, P. Maris, J. P. Vary and A. Abd El-Hady, Phys. Rev. C93, 055202 (2016); arXiv: 1602.06027

Heavy Quarkonium in Holographic basis:

Y. Li, P. Maris, X. Zhao and J. P. Vary, Phys. Letts. B 758, 118 (2016); arXiv:1509.07212

BLFQ Symmetries & Constraints

Baryon number *bi*

Charge *qi*

Angular momentum projection (M-scheme)

Longitudinal momentum (Bjorken sum rule) *xi*

Transverse mode regulator (2D HO) (2*ni*

Global Color Singlets (QCD)

Light Front Gauge

Optional Fock-Space Truncation

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

Light-Front Regularization and Renormalization Schemes

- 1. Regulators in BLFQ (2-D HO params, K)
- 2. Additional Fock space truncations (if any)
- 3. Counterterms identified/tested*
- 4. Sector-dependent renormalization**
- 5. SRG & OLS in NCSM*** adapted to BLFQ (future)

*D. Chakrabarti, A. Harindranath and J.P. Vary, Phys. Rev. D **69**, 034502 (2004) *P. Wiecki, Y. Li, X. Zhao, P. Maris and J.P. Vary, Phys. Rev. D **91**, 105009 (2015)

V. A. Karmanov, J.-F. Mathiot, and A. V. Smirnov, Phys. Rev. D **77, 085028 (2008); Phys. Rev. D **86**, 085006 (2012) **Y. Li, V.A. Karmanov, P. Maris and J.P. Vary, Phys. Letts. B. 748, **278** (2015); arXiv: 1504.05233

***B.R. Barrett, P. Navratil and J.P. Vary, Prog. Part. Nucl. Phys. **69**, 131 (2013)

Positronium

Reglect instantaneous interactions when corresponding dynamical exchange is not present in model space

Exact factorization of CM motion

Preserves Galilean invariance in NCSM and transverse boost invariance in BLFQ

1

$$
H \to H + \lambda_{\text{CM}} H_{\text{CM}}
$$
 with $H_{\text{CM}} = \frac{1}{2} M \Omega^2 R_{\text{CM}}^2$
 $R_{\text{CM}} = 3D$ CM coordinate (NCSM)
 $R_{\text{CM}} = 2D$ transverse CM coordinate (BLFQ)

M. A. Caprio, P. Maris and J. P. Vary, Phys. Rev. C 86, 034312 (2012); arXiv:1208.4156

Y. Li, P.W. Wiecki, X. Zhao, P. Maris and J.P. Vary, Proceedings NTSE-2013, 136 (2014), arXiv: 1311.2980 http://www.ntse-2013.khb.ru/Proc/Yli.pdf

Positronium: P. Weicki, et al., PRD **91**, 105009 (2015)

Consider just second term of effective interaction $\langle f|H_{\text{eff}}^{(2)}(\omega)|i\rangle = \sum_{|n\rangle} \frac{\langle f|H_{01}|n\rangle\langle n|H_{10}|i\rangle}{\omega - E_n}$

• Sum reduces to sum over polarization states of photon

$$
\sum_{\lambda_g} \varepsilon_{\mu}(k_g, \lambda_g) \varepsilon_{\nu}^*(k_g, \lambda_g) = -g_{\mu\nu} + (k_{g,\mu}\eta_{\nu} + k_{g,\nu}\eta_{\mu})/k_g^{\kappa}\eta_{\kappa} \qquad \eta^* = (\eta^*, \eta_{\perp}, \eta^*) = (0, 0_{\perp}, 2) \n\frac{\eta^*}{\eta^2} = \eta^{\mu}\eta_{\mu} = 0
$$

■ Expected cancellation is achieved only if:

$$
\omega = \frac{E_i + E_f}{2}
$$

With this choice the IR divergence of the instantaneous graph is cancelled exactly by IR divergent part of the effective interaction. Henceforward, these cancelling divergences are dropped from the calculations $=$ a counterterm prescription.

Similarly a counterterm is identified and included for the UV divergence in H_{eff} .

Basis Light-Front Quantization (BLFQ) Positronium in QED at Strong Coupling $(\alpha = 0.3)$ Systematic removal of regulators (b = HO momentum scale)

P. Wiecki, Y. Li, X. Zhao, P. Maris and J.P. Vary, Phys. Rev. D **91**, 105009 (2015)

Positronium in QED at Strong Coupling Covariant Basis Light-Front Quantization (BLFQ)

P. Wiecki, Y. Li, X. Zhao, P. Maris and J.P. Vary, Phys. Rev. D **91**, 105009 (2015); & to be published

Consider the case of heavy quarkonium: charmonium and bottomonium

▶ Fock sector truncation, effective Hamiltonian method etc [Wilson '74]

However, this is only suitable for QCD at short distance (and QED).

 \blacktriangleright For long-distance physics, we adopt a confining potential inspired by light-front holographic QCD [Brodsky '06, Trawiński '14]

$$
V(\zeta_{\perp}) = \kappa^4 \zeta_{\perp}^2 + \text{const.} \qquad (\zeta_{\perp} = \sqrt{x(1-x)}r_{\perp})
$$

- \blacktriangleright AdS/QCD: first approximation to QCD inspired by AdS/CFT
- \triangleright soft-wall AdS/QCD produces Regge trajectory [Karch '06]
- I LF holography relates AdS/QCD to LF Schrödinger equation
- Successful applications: spectrum, form factors, β -function, ...

Basis Representation [YL et al., Phys.Lett.B 758, 118 (2016)]

The Hamiltonian is analytically solvable without the one-gluon exchange:

- **Figure 1** Transverse: 2D HO in holographic variables $\phi_{nm}(\vec{k}_{\perp}/\sqrt{x(1-x)})$
- ▶ Longitudinal: $\chi_{\ell}(x) = x^{\frac{1}{2}\alpha}(1-x)^{\frac{1}{2}\beta}P_{\ell}^{(\alpha,\beta)}(2x-1)$
- $\alpha = 2m_{\bar{q}}(m_q+m_{\bar{q}})/\kappa^2$, $\beta = 2m_q(m_q+m_{\bar{q}})/\kappa^2$, $P_\ell^{(a,b)}(z)$ Jacobi polynomials
- \blacktriangleright Mass eigenvalues: $M_{nm\ell}^2 = (m_q + m_{\bar{q}})^2 + 2\kappa^2(2n + |m| + \ell + 3/2) + \frac{\kappa^4}{(m_q + m_{\bar{q}})^2}\ell(\ell+1)$

We adopt these functions (soft-wall LFWFs) as the basis:

$$
\psi_{h/q\bar{q}}(\vec{k}_\perp,x,s,\bar{s})=\!\!\!\!\!\!\sum_{n,m,l}\!\!\Psi_{h/q\bar{q}}(n,m,l,s,\bar{s})\,\phi_{nm}\Big(\frac{\vec{k}_\perp}{\sqrt{x(1\!-\!x)}}\Big)\chi_l(x)
$$

- \triangleright implement LF holographic QCD for first approximation
- transverse 2D HO functions are scalable in the many-body sector $(factorization of c.m. motion)$ [Li '13]
- \blacktriangleright basis truncation: $2n + |m| + 1 \leq N_{\text{max}}$, $l \leq L_{\text{max}}$
- quantum number identification (esp. mirror parity) [Soper '72]

We fix α_s and fit κ , m_q to the experimentally measured masses.

Mass Spectroscopy [YL et al., Phys.Lett.B 758, 118 (2016)]

Light-Front Wavefunctions (LFWFs)

LFWFs provides intrinsic information of the structure of hadrons:

▶ Form factors (electromagnetic, gravitational ...) [Ji '97&'98]

$$
A(q^2) = \sum_{n} \int dD_n \sum_{f=1}^{n} x_f \, \psi_n^* (\{\vec{k}'_{i\perp}, x_i, \lambda_i\}_f) \psi_n(\{\vec{k}_{i\perp}, x_i, \lambda_i\}_f)
$$

$$
\vec{k}'_{i\perp} = \begin{cases} \vec{k}_{i\perp} + (1 - x_i)\vec{q}_{\perp}, & \text{for struck partons} \\ \vec{k}_{i\perp} - x_i \vec{q}_{\perp}, & \text{for spectators.} \end{cases}
$$

In Distributions (hadron tomography) and a state of the Ui '97&'98]

Charge Radii

[YL et al., Phys. Lett. B **758,** 118 (2016); [JPV et al., Few Body Sys. DOI 10.1007/s00601-016-1117-x (2016)]

The charge radius:

$$
\langle r^2 \rangle = -6 \frac{\partial}{\partial Q^2} G_0(Q^2) \big|_{Q^2 \to 0.}
$$

test long-distance physics (cf. decay constants)

Hadron Tomography [Adhikari et al., Phys.Rev.C 93, 055202 (2016)]

- ▶ Generalized parton distributions (GPDs) [Ji '97 & '98] $H(x,\zeta,t)=\frac{1}{2}$ $\int dx^{-}$ 2π $e^{ixP^+z^-}\langle P'|\overline{\psi}(-\frac{1}{2}z)\gamma^+\psi(+\frac{1}{2}z)|P\rangle$ $\overline{}$ $\overline{}$ $|z+z+z=0$ $q = P' - P$, $\zeta = q^+/P^+$, $t = q^2$.
	- \triangleright DVCS, SIDIS, ..., spin physics
- Impact parameter dependent GPDs: [Burkardt '01]

$$
f_{\rm{max}}=f_{\rm{max}}=f_{\rm{max}}
$$

$$
q(x,\vec{b}_{\perp}) = \int \frac{\mathrm{d}^2 \Delta_{\perp}}{(2\pi)^2} e^{i\vec{\Delta}_{\perp} \cdot \vec{b}_{\perp}} H(x,\zeta=0,t=-\Delta_{\perp}^2).
$$

 \blacktriangleright partonic interpretation: $\int d^2b_\perp \int_0^1 dx \left| q(x,\vec{b}_\perp) \right|$ $\vert^{2}=1.$

Decay Constants

[YL et al., Phys.Lett.B 758, 118 (2016)]

- Test "wavefunction at the origin" (cf. charge radius)
- Results are in reasonable agreement with experimental measurements as well as Lattice and DSE calculations where available.
- Results were extrapolated from $N_{\text{max}} = L_{\text{max}} = 8, 16, 24$, and there is some residual regulator dependence.

- Provides access to excited states that are well constrained by \blacktriangleright physical observables (mass spectrum, decay constant etc).
- ▶ BLFQ LFWFs could help to discern the advantages and limitations of the dipole models (GBW, IP-Sat, b-CGC etc).
- ▶ Beyond Eikonal approximation using tBLFQ with Color Glass Condensate [Li, in progress

Generalization to Baryons [work in progress]

The effective interaction can be generalized to the baryon sector:

$$
H_{\text{eff}} = \sum_{a} \frac{\vec{p}_{a\perp}^2 + m_a^2}{x_a} - \vec{P}_{\perp}^2 + \frac{1}{2} \sum_{a,b} V_{ab}^{(2)} + \frac{1}{6} \sum_{a,b,c} V_{abc}^{(3)} + \cdots
$$

The soft-wall confinement: $V_{\text{env}} = \frac{1}{2} \sum_{a} x_a (r_a - \vec{r}_{a\perp})^2$

The soft-wall confinement: $V_{\text{sw}} = \frac{1}{2}$ 2 *a,b* $x_a x_b (\vec{r}_{a\perp} - \vec{r}_{b\perp})^2$.

 \blacktriangleright The one-gluon exchange

Jacobi coordinates on the light front (three-body example): longitudinal: $x = x_3$, $\chi = \frac{x_2}{1 - x_3}$; ${\rm transverse\,\,momenta:}\,\,\,\vec{k}_{\perp}=(1-x_3)\vec{p}_{3\perp}-x_3(\vec{p}_{1\perp}+\vec{p}_{2\perp}),\,\,\,\,\,\,\vec{\kappa}_{\perp}=\frac{x_1\vec{p}_{2\perp}-2\vec{p}_{1\perp}}{x_1+x_2};$ transverse coordinates: $\vec{r}_{\perp} = \vec{r}_{3\perp} - \frac{x_1\vec{r}_{1\perp} - x_2\vec{r}_{2\perp}}{x_1+x_2}, \quad \vec{\rho}_{\perp} = \vec{r}_{1\perp} - \vec{r}_{2\perp}.$

- \blacktriangleright Taking advantage of the kinematical nature of light-front boosts $V_{\text{sw}} = \kappa^4 x (1-x) \vec{r}_{\perp}^2 + \kappa^4 (1-x) \chi (1-\chi) \vec{\rho}_{\perp}^2$
- \blacktriangleright The longitudinal confinement $V_L = -\frac{\kappa^4}{(m_1+m_2+m_3)^2}$ $\sqrt{ }$ $\partial_x(x(1-x)\partial_x) + \frac{1}{1-x}$ $\partial_{\chi} (\chi(1-\chi) \partial_{\chi})$ $\overline{}$

Emergent Phenomena

NCSM: Clustering and Collective Rotational Motion BLFQ: Spontaneous Symmetry Breaking

9Be Translationally invariant gs density Full 3D densities = rotate around the vertical axis

C. Cockrell, J.P. Vary, P. Maris, Phys. Rev. C86, 034325 (2012); C. Cockrell, PhD, Iowa State University

Can we observe a phase transition in Φ_{1+1}^4 ?

How does a phase transition develop as a function of increased coupling? What are the observables associated with a phase transition?

What are its critical properties (coupling, exponent, ...)?

ϕ^4 in 1+1 Dimensions DLCQ with Coherent State Analysis

- **A.** Derive the Hamiltonian and quantize it on the light front, investigate coherent state treatment of vacuum: A. Harindranath and J.P. Vary, Phys Rev D**36**, 1141(1987)
- **B.** Obtain vacuum energy as well as the mass and profile functions (topological properties) of soliton-like solutions ("Kinks") in the symmetry-broken phase:

APBC: $SSB = degeneracy \sim Kink \sim coherent state!$ Chakrabarti, Harindranath, Martinovic and Vary, Phys. Letts. B**582**, 196 (2004); hep-th/0309263

PBC: $SSB = degeneracy \sim Kink + Antinkink \sim coherent state!$ Chakrabarti, Harindranath, Martinovic, Pivovarov and Vary, Phys. Letts. B**617**, 92(2005); hep-th/0310290.

C. Demonstrate onset of Kink Condensation at strong coupling (**APBC**) Chakrabarti, Harindranath and Vary, Phys. Rev. D**71**, 125012(2005); hep-th/0504094

D. Chakrabarti, A. Harindranath and J.P. Vary, *Phys. Rev. D* **71**, 125012(2005); hep-th/05104094.

D. Chakrabarti, A. Harindranath and J.P. Vary, *Phys. Rev. D* **71**, 125012(2005); hep-th/05104094.

Compare lowest state's LF momentum distribution at strong coupling with ansatz variational coherent state' s

D. Chakrabarti, A. Harindranath and J.P. Vary, *Phys. Rev. D* **71**, 125012(2005); hep-th/05104094.

At weak coupling, kink-boson scattering states and kink collective excitation observed

State 9 => 2 boson excitation

D. Chakrabarti, A. Harindranath and J.P. Vary, *Phys. Rev. D* **71**, 125012(2005); hep-th/05104094.

Compare lowest state's topology at strong coupling with ansatz variational coherent state topology

D. Chakrabarti, A. Harindranath and J.P. Vary, *Phys. Rev. D* **71**, 125012(2005); hep-th/05104094.

Continuum limit of the critical coupling and critical exponent D. Chakrabarti, A. Harindranath and J.P. Vary, *Phys. Rev. D* **71**, 125012(2005); hep-th/05104094.

Analysis of the vanishing mass gap $δM²$ yields:

 $\boldsymbol{\delta M}^2 = \left(\left| \boldsymbol{\lambda} - \boldsymbol{\lambda}_c \right| \right)^{\nu}$

Agrees with classical constructive field theory

tBLFQ: Nonlinear Compton Scattering

See Friday's talk by Xingbo Zhao

• Space-time structure

• Two effects: acceleration and radiation

Xingbo Zhao, Anton Ilderton, Pieter Maris and James P. Vary, Phys. Rev. D 88, 065014 (2013); and Phys. Letts B 726, 856 (2013); Guangyao Chao, et al, in preparation

Summary and Outlook

There exist multiple avenues of symbiosis between ab initio nuclear theory and relativistic quantum field theory

Continuous interchange should be mutually beneficial:

 \blacklozenge Many-body theory – bound states and scattering !Renormalization, regularization and extrapolation ◆ Uncertainty quantification !Methods for identifying emergent phenomena ◆ Efficient utilization of supercomputing resources

This INT program is one example of a productive approach