

Light-front approach to hadron structures with quantum computing

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 - Results of observables

Introduction to Quantum Computing

- * **Classical computers:**
 - classical bit: 0, 1 _
 - implementation: electric voltage Low, High
 - classical gates: AND, OR, NOT, Bitwise logic gates
 - deterministic nature

- Quantum computers: *
- quantum bit (qubit): $|0\rangle = {1 \choose 0}, |1\rangle = {0 \choose 1}$
- implementation: two-level quantum systems

 $|\Psi\rangle = \alpha |0\rangle + \beta |1\rangle, \ |\alpha|^2 + |\beta|^2 = 1$

- quantum gates: unitary operators
- superposition
- states only collapse when measured
- can theoretically solve problems classical computers cannot solve









Developments in Quantum Computing

Quantum computing has come a long way in past 40 years

- Quantum implementation of Toffoli Gate (1980)
- Deutsch-Jozsa Algorithm: First example of quantum algorithm that is exponentially faster (1992)
- <u>Shor's Algorithm:</u> Factoring large numbers (1994)
- Quantum Error Correction (1995)
- Transmon Qubits (2007)
- <u>Variational Quantum Eigensolver</u>: broad applications in quantum chemistry (2014)
- <u>Quantum Machine Learning</u>: Quantum classifier, Quantum Support Vector Machines, Quantum Approximation Optimization, etc (2017)

Noisy Intermediate-Scale Quantum (NISQ): those devices whose qubits and [Preskill, 2018] quantum operations are substantially imperfect. [Bharti, 2101.08448]

Quantum advantage: a purpose-specific computation that involves a quantum device and that can not be performed classically with a reasonable resources. [Google AI, Arute 2019] [UTSC, Zhong 2020]

Major areas of quantum computing applications include:

- Quantum Fourier transform (quantum arithmetic, phase estimation)
- Quantum search algorithm (Grover's algorithm)
- **Quantum simulations** (VQE, QAOA)



Why are we interested?

"Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical" (Richard Feynman)

Many problems are inherently quantum mechanical.

- <u>Vast amount of encoded information</u> in a many-qubit state: the total state space of n-qubit goes with 2^n
- High <u>scalability</u> in quantum applications (compact encoding)
- Many-body problems and quantum computing are similar by nature
- Rapid progress in <u>quantum hardware</u>
 (~100 qubits, improved scale, quality and speed)
 [IBM, 2110.14108]



Light-front Hamiltonian formalism



Basis Light-front Quantization (BLFQ)

 Basis function approach exploit symmetry

In the application of the light mesons within the valence $\ket{qar{q}}$ Fock sector



 $m_q \, (m_{ar q})$ is the mass of the quark/antiquark, κ is the confining strength V_g is the one-gluon exchange, H_{γ_5} is the pseudoscalar contact interaction [Li, 1704.06968]

[Vary, 0905.1411]



front form

Light meson spectrum and wave functions

Transverse and longitudinal basis functions are truncated with N_{max} (basis energy scale) and L_{max} (longitudinal resolution) for the <u>light-front wave functions</u> (LFWFs) :



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QCD evolutions

- Parton distribution function (PDF): we used DGLAP equations to evolve our initial PDF to experimental scale.
 [Dokshitzer, 1977]
- Parton distribution amplitude (PDA): we used ERBL equations for the PDA evolution.
 [Lepage, 1980]



E615 data [Conway, 1989]

Initial scale $\mu_0 = 0.56 \text{ GeV} \pm 5\%$

E791 data [Aitala, 2001]



Variational Quantum Eigensolvers (VQE)

VQE is directly inspired by the variational principle.

The core idea is to use a **parameterized unitary ansatz** (educated guess that produces the "trial wave function") to obtain the lowest eigenvalue via continuous optimizations.





[Peruzzo, 1304.3061] [Nakanishi, 1810.09434]

Adapting problem to quantum computers



For an initial application on quantum computers (or simulators), we truncate our basis functions at $(N_{\text{max}}, L_{\text{max}}) = (1, 1)$ and $(N_{\text{max}}, L_{\text{max}}) = (4, 1)$. [Qian, 2112.01927]

	$N_{ m f}$	$lpha_{ m s}(0)$	κ (MeV)	$m_q \; ({\rm MeV})$	$N_{ m max}$	L_{\max}	Matrix dimension
$H_{ m eff}^{(1,1)}$	3	0.89	560 ± 10	300 ± 10	1	1	4 by 4
$H_{ m eff}^{(4,1)}$					4	1	16 by 16

• <u>Encoding</u>: Jordan-Wigner encoding O(N), compact encoding $O(\log N)$

 $(N,N) = (2^n, 2^n) \rightarrow H_q = \sum_{\alpha} c_{\alpha} P_{\alpha}$ Logarithmic scaling [Jordan & Wigner (1928)] [Kreshchuk, 2002.04016]

- Variational ansatzes: Unitary Coupled Cluster ansatz and Hardware Efficient
 heuristic ansatz.
 [Barkoutsos, 1805.04340] [Kandala, 1704.05018]
- <u>Algorithms:</u> **VQE** for the ground state. **SSVQE** for the full spectroscopy.

[Peruzzo, 1304.3061] [Nakanishi, 1810.09434]

With LFWF on qubits, additional physical observables (like decay constants) are computed *directly* on the quantum circuits.

Hamiltonian and basis encoding



Example of $N_{\max} = L_{\max} = 1$ (smallest Hamiltonian matrix) where matrix element corresponds to $(n, m, l, s, \overline{s})$ basis state,

		$H_{ m eff}^{(1,1)}$	$=\left(\begin{bmatrix} \xi \\ \xi \end{bmatrix} \right)$	$568487 \\ 0 \\ 25428 \\ 0 \\ 0$	$\begin{array}{c} 0 \\ 1700976 \\ 0 \\ -15767 \end{array}$	$25428 \\ 0 \\ 568487 \\ 0$	$\begin{array}{c} 0 \\ -15767 \\ 0 \\ 1700976 \end{array}$	(All units i	in MeV
	n	m	l	s	\overline{s}	Direct	encoding	Compact encoding	
1)	0	0	0	1/2	-1/2	C	$ 0001\rangle$	$ 00\rangle$	
2	0	0	0	-1/2	1/2	C	0010 angle	01 angle	
3)	0	0	1	1/2	-1/2	C	$ 100\rangle$	10 angle	
4	0	0	1	-1/2	1/2	1	$ 000\rangle$	11 angle	

From second quantization, the Hamiltonian can be written in terms of creation and annihilation operators,

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \dots = \sum_{ij} h_{ij} \hat{a}_i^{\dagger} \hat{a}_j + \frac{1}{4} \sum_{ijkl} h_{ijkl} \hat{a}_i^{\dagger} \hat{a}_j^{\dagger} \hat{a}_k \hat{a}_l + \dots$$

We focus only on the single-body interactions and identify h_{ij} as the Hamiltonian matrix elements.

Qubit encoding

Suppose *H* of dimension $(N, N) = (2^n, 2^n) \rightarrow H_q = \sum_{\alpha} c_{\alpha} P_{\alpha}$

1. <u>Direct encoding</u>: Jordan-Wigner (JW) encoding, basically map directly from using the 2 x 2 Pauli spin matrices $\sigma_k \in \{I_k, X_k, Y_k, Z_k\}$.

$$\hat{a}_{j}^{\dagger} = \bigotimes_{i=1}^{j-1} Z_{i} \otimes \frac{X_{j} - iY_{j}}{2} \qquad H_{\text{direct}}^{(1,1)} = 2269462 \text{ IIII} - 284243 \text{ (ZIII + IIZI)} \\ - 850488 \text{ (IZII + IIIZ)} + 12714 \text{ (XZXI + YZYI)} \\ - 7883 \text{ (IXZX + IYZY)}, \qquad (Kreshchuk, 2002.04016)$$

2. <u>Compact encoding</u>: utilize orthogonal basis formed by Pauli strings $P_{\alpha} = \bigotimes_{k=1}^{n} \sigma_{k}$ under trace, one can further reduce the *N*-by-*N* Hamiltonian (Hilbert-Schmidt inner product space) $O(\log N) = O(n)$

$$H_q = \frac{1}{N} \sum_{\alpha=1}^{N^2} \operatorname{Tr}(P_{\alpha}H) \cdot P_{\alpha}$$

$$H_{\text{compact}}^{(1,1)} = 1134731 \,\text{II} - 566245 \,\text{IZ} \\ + 4831 \,\text{XI} + 20598 \,\text{XZ}$$



[Jordan and Wigner (1928)]

[Nielson (2000)]

Variational ansatz $\hat{U}(\vec{\theta})$



Variational ansatz is an <u>educated guess</u> of the unitary circuit with parameters to be optimized in each iteration.



- 2. Hardware efficient (HE) ansatz [Kandala, 1704.05018]
- heuristic ansatz
- consists of alternating single-qubit rotations and entangling blocks (repetition layers)
- proven to work for general problems



EfficientSU2 ansatz with 1 repetition layer [Qiskit 0.32.1 library]

Optimization algorithms



Variational Quantum Eigensolver (VQE) algorithm finds ground state

[Peruzzo, 1304.3061]



Subspace-search VQE (SSVQE) algorithm finds excited states

In particular, Weighted SSVQE for up to k-th excited states [Nakanishi, 1810.09434]



 $ec{\omega}$ is a strictly decreasing weight vector prioritizing lower-lying states

For example: $C_{\vec{\omega}}(\vec{\theta}) = E_0 + 0.5E_1 + 0.25E_2$, $\vec{\omega} = (1, 0.5, 0.25)$

Results: VQE $(N_{\max}, L_{\max}) = (1, 1)$





- IBM simulators + backends:
- <u>statevector (SV) simulator</u> (noise-free exact simulation)
- <u>qasm simulator</u> (sampling noise from 8192 shots per measurement)

- [Qiskit 0.32.1 library]
- IBMQ manila (5 Qubits, 32 QV, 2.8K CLOPS, 2e-2% readout error, 8192 shots per measurement)



Results: SSVQE $(N_{\max}, L_{\max}) = (1, 1)$



- Both use <u>compact encoding with HE ansatz</u> (2 repetition layers, 12 params)
- Cost function:

 $1.0 \cdot E_{|00\rangle} + 0.5 \cdot E_{|01\rangle} + 0.25 \cdot E_{|10\rangle} + 0.125 \cdot E_{|11\rangle}$

• Note:

Spectrum always <u>emerge in accordance</u> with the specified weight order.

Results: SSVQE $(N_{\max}, L_{\max}) = (4, 1)$



- Low-lying spectrum (lowest 4 states instead of 16 possible states)
- Both use <u>compact encoding with HE ansatz</u> (6 repetition layer, 53 params)

Results: decay constants



Decay constants are defined as vacuum-to-hadron matrix element of the quark current operator. In BLFQ basis, we write the decay constants as:

$$f_{\rm P,V} = 2\sqrt{2N_c} \int_0^1 \frac{\mathrm{d}x}{2\sqrt{x(1-x)}} \int \frac{\mathrm{d}^2 \mathbf{k}_\perp}{(2\pi)^3} \psi_{\uparrow\downarrow\mp\downarrow\uparrow}^{(m_j=0)}(x, \mathbf{k}_\perp)$$

$$\equiv \frac{\kappa\sqrt{N_c}}{\pi} \sum_{nl} (-1)^n C_l(m_q, \kappa) \left(\tilde{\psi}_{\uparrow\downarrow}^{(m_j=0)}(n, 0, l) \mp \tilde{\psi}_{\downarrow\uparrow}^{(m_j=0)}(n, 0, l)\right)$$
[Li, 1704.06968]

In the VQE/SSVQE, the light-front wave function (LFWF) is encoded on the qubits. One can **directly** compute observables such as decay constants on the quantum circuit:

$$f_{\rm P,V} \propto |\langle \nu_{\rm P,V} | \psi(\vec{\theta}) \rangle| = \sqrt{\langle \psi(\vec{\theta}) | (|\nu_{P,V} \rangle \langle \nu_{P,V} |) | \psi(\vec{\theta}) \rangle}$$

For example, in $(N_{\max}, L_{\max}) = (1, 1)$

$$\nu_{\rm P}^{(1,1)} = (1,-1,0,0) \qquad \longrightarrow \qquad |\nu_{P,V}^{(1,1)}\rangle \langle \nu_{P,V}^{(1,1)}|_q = 0.5 \left(II \mp IX + ZI \pm ZX\right)$$

Results: decay constants



Summary of decay constants for the lowest two states (π and ρ mesons). Experimental decay constants are around 130 MeV and 216 MeV, respectively.

[Zyla, 2020]

$N_{\rm max}$	L_{\max}	Decay constants	Exact result (MeV)	SV sim (MeV)	qasm sim (MeV)
1	1	$f_{\pi} \ f_{ ho}$	178.18 178.18	178.18 178.18	178.17 ± 1.97 178.17 ± 1.97
4	1	$f_{\pi} \ f_{ ho}$	193.71 231.00	193.32 232.93	194.28 ± 15.49 225.72 ± 13.44

Uncertainty (sampling error) in qasm simulator results from measurements of 8192 shots.

Results: parton distribution functions



Parton distribution functions (PDFs) is the probability of finding a particle with longitudinal momentum fraction x under some factorization scale related to experimental conditions,

$$q(x;\mu) = \frac{1}{x(1-x)} \sum_{s\bar{s}} \int \frac{\mathrm{d}^2 \mathbf{k}_{\perp}}{2(2\pi)^3} |\psi_{s\bar{s}}^{(m_j=0)}(x,\mathbf{k}_{\perp})|^2 \qquad \text{[Li, 1704.06968]}$$
$$\equiv \frac{1}{4\pi} \sum_{s\bar{s}} \sum_{nm} \sum_{l\bar{l}} \tilde{\psi}_{s\bar{s}}^{*(m_j=0)}(n,m,\bar{l}) \tilde{\psi}_{s\bar{s}}^{(m_j=0)}(n,m,l) \chi_l(x) \chi_{\bar{l}}(x)$$

Using projection operators, one can **<u>directly</u>** compute the PDF on quantum computers as well. Note: PDF operator on qubits depends on *x*.

$$q(x) = \sum_{s\bar{s}} \sum_{nm} \sum_{l\bar{l}} \left\langle \psi(\vec{\theta}) \right| \hat{O}_{\rm pdf}(x) \left| \psi(\vec{\theta}) \right\rangle$$

Qubitized operators:

$$\hat{O}_{\rm pdf}(x) = \hat{U}_{\rm p}(s,\bar{s},n,m,\bar{l})^{\dagger} \hat{U}_{\rm p}(s,\bar{s},n,m,l) \chi_l(x) \chi_{\bar{l}}(x) / 4\pi$$

$$\hat{O}_{\rm pdf}^{(1,1)}(0.5)_q = 1.30\,II - 1.29\,IX - 0.18\,IZ, \qquad \hat{O}_{\rm pdf}^{(1,1)}(0.25)_q = 0.78\,\left(II + IZ\right).$$

Results: parton distribution functions



- In both basis truncations, the PDFs for lowest two states are comparable due to the lack of longitudinal excitations.
- For $(N_{\max}, L_{\max}) = (1, 1)$, qasm results agree with exact calculations.
- For $(N_{\max}, L_{\max}) = (4, 1)$, PDF is rescaled due to lack of normality of the PDF/LFWF at this cutoff.



Radiative transitions (Preliminary)

The electromagnetic transition between two hadron states is governed by the hadron matrix element, which is key to calculating the transition form factor & decay width (probe the internal structure of QCD bound state):

$$I^{\mu}_{m'_j,m_j} = \langle \psi_B(p',j',m'_j) | J^{\mu}(x) | \psi_A(p,j,m_j) \rangle$$

For example, a physical process between a vector meson (V) and a pseudoscalar (P), $\,{\rm V}\to{\rm P}+\gamma$

The SSVQE approach allows one to compute any transition amplitude by using a <u>superposition</u> of the incoming and outgoing meson states. [Nakanishi, 1810.09434]

$$A = \langle \psi_i(\vec{\theta}) | \hat{A} | \psi_j(\vec{\theta}) \rangle = \langle \psi_i | U^{\dagger}(\vec{\theta}) \hat{A} U(\vec{\theta}) | \psi_j \rangle$$

$$\operatorname{Re}(A) = \langle \psi_{ij}^{+x} | U^{\dagger}(\vec{\theta}) \hat{A} U(\vec{\theta}) | \psi_{ij}^{+x} \rangle - \frac{1}{2} \Big(\langle \psi_i | U^{\dagger}(\vec{\theta}) \hat{A} U(\vec{\theta}) | \psi_i \rangle + \langle \psi_j | U^{\dagger}(\vec{\theta}) \hat{A} U(\vec{\theta}) | \psi_j \rangle \Big)$$

$$\operatorname{Im}(A) = \langle \psi_{ij}^{+y} | U^{\dagger}(\vec{\theta}) \hat{A} U(\vec{\theta}) | \psi_{ij}^{+y} \rangle - \frac{1}{2} \Big(\langle \psi_i | U^{\dagger}(\vec{\theta}) \hat{A} U(\vec{\theta}) | \psi_i \rangle + \langle \psi_j | U^{\dagger}(\vec{\theta}) \hat{A} U(\vec{\theta}) | \psi_j \rangle \Big)$$

$$\psi_A$$
 ψ_B

[M Li, 1803.11519]

$$|\psi_{ij}^{+x}\rangle = \frac{1}{\sqrt{2}}(|\psi_i\rangle + |\psi_j\rangle)$$

$$|\psi_{ij}^{+y}\rangle = \frac{1}{\sqrt{2}}(|\psi_i\rangle + i |\psi_j\rangle)$$



Radiative transitions (Preliminary)



<u>Initial quantum circuits</u> for calculating Re(A) or Im(A) can be constructed with only X, H, S, CX gates. Switching H with S-H-S gates to calculate Im(A).



Summary and outlook



We presented two promising quantum computing approaches, <u>VQE and SSVQE</u>, to find <u>meson spectroscopy and observables</u> on the light front for the light meson system.

Basis light-front quantization approach (BLFQ) works well with the VQE and SSVQE approaches.

Future plans:

- Optimize the VQE and SSVQE programs to solve the original Hamiltonian and compute on real quantum backends. $N_{\max} = 8, L_{\max} = 1 \Rightarrow (32, 32)$ Hamiltonian => 5 qubits $N_{\max} = 8, L_{\max} = 3 \Rightarrow (64, 64)$ Hamiltonian => 6 qubits
- Calculations on transition matrix element of an operator using SSVQE approach.
 Take advantage of <u>quantum superposition</u>!
- Investigation into other **many-body** QCD bound state problems.

Backup slides

Light-front dynamics





Simplifies the dispersion relation

$$P^0 = \sqrt{m^2 + \vec{P}} \implies P^- = (m^2 + \mathbf{P}_{\perp}^2)/P^+$$

- One more kinematical variable
- Light-front vacuum is trivial (we ignore zero mode)

LF time: $x^+ = x^0 + x^3$ LF energy: $P^- = P^0 - P^3$ LF longitudinal momentum: $P^+ = P^0 + P^3$ LF transverse momentum: $\mathbf{P} \equiv \vec{P}^{\perp} = (P^1, P^2)$

Light mesons Hamiltonian in detail



Light-front Hamiltonian in $|q \bar{q} \rangle$:



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

- 1. Light-front Kinetic energy
- 2. Confinement:

(a) Transverse holographic confinement [Brodsky, 2015]

- (b) Longitudinal confinement [Li, 2016]
- 3. One-gluon exchange with running coupling [Krautgartner, 1992] $V_{a} = -\frac{4}{2} \frac{4\pi \alpha_{s}(Q^{2})}{\bar{\mu}_{a'}} \bar{\mu}_{a'}(\mathbf{k}', x') \gamma_{\mu} \mu_{a}(\mathbf{k}, x) \bar{\nu}_{\bar{a}}(-\mathbf{k}, 1-x) \gamma^{\mu} \nu_{\bar{a}'}(-\mathbf{k}')$

$$V_g = -\frac{4}{3} \frac{4\pi \alpha_{\rm s}(Q^{-})}{Q^2} \bar{u}_{s'}(\mathbf{k}_{\perp}', x') \gamma_{\mu} u_s(\mathbf{k}_{\perp}, x) \bar{v}_{\bar{s}}(-\mathbf{k}_{\perp}, 1-x) \gamma^{\mu} v_{\bar{s}'}(-\mathbf{k}_{\perp}', 1-x')$$

4. Point-like pseudoscalar interaction [Inspired by Jia, 2019 & Mannheim, 2017] 24 = 25 + 4 = 25 + 4 = 25 + 4 = 25

$$\mathcal{H}_{\gamma_5} = \lambda \bar{\psi}(x) \gamma^5 \psi(x) \bar{\psi}(x) \gamma^5 \psi(x)$$

General approach to the entire light meson sector with simplification of isospin and charge

Basis functions in detail



Basis functions [Li, 2016; 2017]

relative-particle coordinate

$$\psi_{s\bar{s}/h}(\mathbf{k}_{\perp}, x) = \sum_{n,m,l} \psi_h(n,m,l,s,\bar{s})\phi(\mathbf{k}_{\perp}/\sqrt{x(1-x)})\chi_l(x)$$
(2D HO functions)

- Transverse:
$$\phi_{nm}(\mathbf{q}_{\perp}) = \frac{1}{\kappa} \sqrt{\frac{4\pi n!}{(n+|m|)!} \left(\frac{q_{\perp}}{\kappa}\right)^{|m|}} e^{-\frac{1}{2}q_{\perp}^2/\kappa^2} L_n^{|m|}(q_{\perp}^2/\kappa^2) e^{im\theta_q}$$

- Longitudinal: $\chi_l(x;\alpha,\beta) = \sqrt{4\pi(2l+\alpha+\beta+1)}\sqrt{\frac{\Gamma(l+\alpha+\beta+1)}{\Gamma(l+\alpha+1)(\Gamma(l+\beta+1))}}x^{\frac{\beta}{2}}(1-x)^{\frac{\alpha}{2}}P_l^{(\alpha,\beta)}(2x-1)$

(Jacobi polynomials)

where
$$\alpha = 2m_{ar{q}}(m_q+m_{ar{q}})/\kappa^2, \beta = 2m_q(m_q+m_{ar{q}})/\kappa^2$$

- Basis truncations $2n + |m| + 1 \le N_{\max}$ $l \le L_{\max}$
- Cutoff and resolution $\Lambda_{\rm uv} \approx \kappa \sqrt{N_{\rm max}} \qquad \lambda_{\rm IR} \approx \kappa / \sqrt{N_{\rm max}} \qquad \Delta x \approx L_{\rm max}^{-1}$

This model serves as first step to the light meson sector with BLFQ, and provides access to the full spectroscopy.

Spectroscopy





H_{eff}	3	0.89	$610(5)^{*}$	480 (5) *	11	8	24	-	127
$H_{{ m eff},\gamma_5}$	U	0.07	010(0)	100 (0)		0	2.	0.56(1)*	111

between PDG and BLFQ for the 11 identified states.

[Qian, 2005.13806]

Spectroscopy comparison



Comparison with experimental data and other model calculations (in GeV). Fitted masses are labeled with red asterisks.

	j	Р	С	PDG	$\mathrm{AdS}/\mathrm{QCD}$	BSE	BLFQ $(H_{\text{eff},\gamma_5})$ (This work)
$\pi(140)$	0	-	+	0.14	0.14 *	0.14 (0.14) *	0.14 *
$\rho(770)$	1	—	-	0.78	0.78	0.76 (0.74)	0.78 *
$a_0(980)$	0	+	+	0.98	0.78	0.64(1.1)	0.74
$b_1(1235)$	1	+	-	1.23	1.09	0.85(1.3)	1.20
$a_1(1260)$	1	+	+	1.23	1.09	0.97(1.3)	1.09
$\pi(1300)$	0	-	+	1.30	1.09	1.10	1.44
$a_2(1320)$	2	+	+	1.32	1.33	1.16	1.34
$\rho(1450)$	1	-	+	1.45	1.33	1.02	1.44 *
$a_0(1450)$	0	+	+	1.47	1.33	1.27	1.65
$\pi_2(1670)$	2	1000	+	1.67	1.53	1.23	1.59
$\rho_{3}(1690)$	3	—	+	1.69	1.71	1.54	1.69
				(r.m.s.)	127 MeV	275 (220) Me	V 111 MeV

[Qian, 2005.13806]

Light-Front Wavefunction (LFWF)

LFWFs (as eigenvectors) are also obtained. This is a key advantage of Hamiltonian formalism, which enables us to compute physical observables. [Qian, 2005.13806]



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Comparison with other systems. Dominant wavefunctions(singlet) for pseudoscalar mesons from heavy to light systems:



[Y. Li, 1704.06968] [Qian, 2005.13806]

Comparison of LFWF spin components:









Quantum circuit basics



- Each horizontal line represents the evolution of a qubit (from left to right)
- Each measurement collapses the wave function and we obtain either 0 or 1 in the computation basis
- In practice, measurements are statistical outcomes by running the same circuit repeatedly for thousands of times (or shots)
- Finally, statistical outcomes lead to find the associated expectation value.

Optimizers



Optimizers (on classical computers) aim to minimize the loss functions and updates the parameter for next iteration.

- **COBYLA**: constrained optimization, derivative-free
- **LBFGSB**: quasi-Newton method, derivative-based
- **SPSA**: Simultaneous Perturbation Stochastic Approximation; can handle measurement uncertainty [diagram from Pennylane]
- **QNSPSA**: Quantum Natural SPSA; improve SPSA by sampling natural gradients; significant speed up



More optimizers at scipy.optimize.minimize qiskit.algorithms.optimizers



Detailed statistics of VQE results

Simulator	Encoding	Optimizer	Ground state energy (MeV^2)	Iterations
	Direct	LBFGSB	543059~(0%)	60
\mathbf{SV}	Direct	COBYLA	543059~(0%)	90
	Compact	LBFGSB	543059~(0%)	11
<i>a</i> .	Compact	COBYLA	543059~(0%)	344
	Direct	COBYLA	$552344 \pm 996 \ (1.53\%)$	41
gasm	Direct	SPSA	$545767 \pm 152 \ (0.47\%)$	1051
	Compact	COBYLA	$547405 \pm 211 (0.76\%)$	99
	Compact	SPSA	$543065 \pm 6 (0\%)$	1551
Exact solution	¥ 4	-	543059	-

New result using VQEClient on IBMQ manila: 554568 +/- 1179 (1.90%)



Detailed statistics of SSVQE results

$N_{\rm max}$	L_{\max}	State	Exact energy (MeV^2)	$SV sim (MeV^2)$	qasm sim (MeV^2)
		$ 00\rangle$	543059	543059 (0%)	$543059 \pm 0 \ (0\%)$
1 1	1	$_1 01\rangle$	593915	593915~(0%)	$593915\pm 0~(0\%)$
		$ 10\rangle$	1686541	$1685210 \ (0.08\%)$	$1686541 \pm 70 \ (0\%)$
		$ 11\rangle$	1715577	1716743~(0.07%)	$1715577 \pm 66 \ (0\%)$
		$ 0000\rangle$	180012	$180802 \ (0.44\%)$	$189263 \pm 6511 (1.08\%)$
4	1	$ 0001\rangle$	402071	405796~(0.93%)	$419139 \pm 6324~(1.73\%)$
		$ 0010\rangle$	493293	499376~(1.23%)	$532381 \pm 7008~(5.21\%)$
		$ 0011\rangle$	742530	774189 (4.26%)	$745422\pm 6503~(2.88\%)$



Hamiltonian encoding for $(N_{\max}, L_{\max}) = (4, 1)$

 $H_{\text{compact}}^{(4,1)} = 1868696 IIII - 623614 IIIZ + 518799 IIXI + 44344 IIXZ$ $-531599\,IIZI + 11950\,IIZZ + 29183\,IYIY - 21316\,IYXY$ + 28874 IYYI + 22502 IYYX - 1474 IYYZ + 6301 IYZY+ 1762 XXII + 7092 XXIZ - 310 XXXI - 4214 XXXZ+ 653 XXZI + 3207 XXZZ + 77283 XZII - 61720 XZIX+4548 XZIZ - 38263 XZXI + 33154 XZXX - 3510 XZXZ+ 844 XZYY + 19387 XZZI - 15666 XZZX + 2304 XZZZ+ 29183 YIIY - 21316 YIXY - 28874 YIYI + 22502 YIYX+ 1474 YIYZ + 6301 YIZY + 1762 YYII + 7092 YYIZ-310YYXI - 4214YYXZ + 653YYZI + 3207YYZZ-77283 ZXII - 61720 ZXIX - 4548 ZXIZ + 38263 ZXXI+ 33154 ZXXX + 3510 ZXXZ + 844 ZXYY - 19387 ZXZI-15666 ZXZX - 2304 ZXZZ + 215302 ZZII - 34396 ZZIZ+70683 ZZXI + 19390 ZZXZ - 12936 ZZZI - 11024 ZZZZ,



Basis encoding for $(N_{\max}, L_{\max}) = (4, 1)$

	n	m	l	8	\bar{s}	Compact encoding
1	0	0	0	1/2	-1/2	$ 0000\rangle$
(2)	0	0	0	-1/2	1/2	0001 angle
3	0	0	1	1/2	-1/2	$ 0010\rangle$
(4)	0	0	1	-1/2	1/2	$ 0011\rangle$
(5)	0	1	0	-1/2	-1/2	$ 0100\rangle$
6	0	1	1	-1/2	-1/2	0101 angle
(7)	0	-1	0	1/2	1/2	$ 0110\rangle$
8	0	-1	1	1/2	1/2	0111 angle
9	1	0	0	1/2	-1/2	$ 1000\rangle$
(10)	1	0	0	-1/2	1/2	1001 angle
(11)	1	0	1	1/2	-1/2	$ 1010\rangle$
(12)	1	0	1	-1/2	1/2	$ 1011\rangle$
	1	1	0	-1/2	-1/2	$ 1100\rangle$
$\overline{14}$	1	1	1	-1/2	-1/2	1101 angle
$\overline{(15)}$	1	-1	0	1/2	1/2	$ 1110\rangle$
$\underbrace{16}$	1	-1	1	1/2	1/2	$ 1111\rangle$