

# Light front approach to hadrons on quantum computers

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#### Outline

- 1. Introduction to quantum computing
  - Recent developments
  - Variational quantum eigensolvers
- 2. Application to nuclear bound states: light mesons
  - Effective light-front Hamiltonian
  - Meson spectroscopy
  - Observables
- 3. Summary and outlook



# 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)

[Preskill, 2018]

**Noisy Intermediate-Scale Quantum (NISQ)**: those devices whose qubits and 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]

- Sampling pseudo-random quantum circuit with 53-qubit Sycamore superconducting chip
- Gaussian boson sampling with Jiuzhang photonic quantum computer [UTSC, Zhong 2020]

Our application: Variational Quantum Eigensolver (VQE) and Subspace-search VQE (SSVQE) approaches to hadronic bound-state problems on the light front

# VQE is a hybrid algorithm

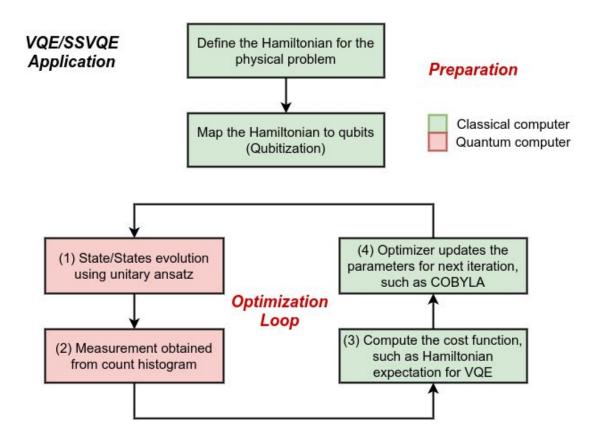


[Peruzzo, 1304.3061]

VQE is directly inspired by the variational principle.

[Nakanishi, 1810.09434]

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



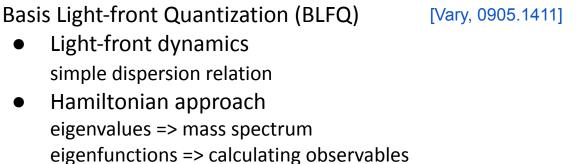


# Why are we interested in quantum computing?

- "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.
- Vast amount of encoded information in a many-qubit state: the total state space of *n*-qubit goes with 2<sup>n</sup>
- High scalability in quantum applications (compact encoding)
- Many-body problems and quantum computing are similar by nature
- Rapid progress in quantum hardware (~100 qubit capability)

# Effective model of light mesons

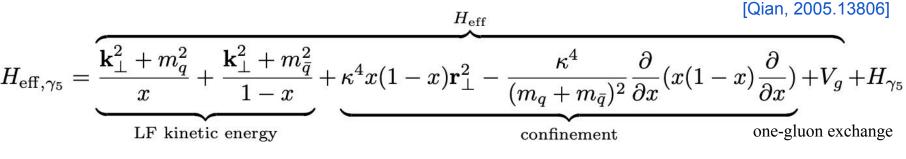




 Basis function approach exploit symmetry; discretize the Hamiltonian

front form

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,  $\kappa$  is the confining strength  $V_g$  is the one-gluon exchange,  $H_{\gamma_5}$  is the pseudoscalar contact interaction [Li, 1704.06968]

# Effective model of light mesons



Transverse and longitudinal basis functions are truncated separately with  $N_{\text{max}}$  (basis energy scale) and  $L_{\text{max}}$  (longitudinal resolution):

$$\psi_{s\bar{s}}^{m_j}(\boldsymbol{k}_{\perp}, x) = \sum_{nml} \tilde{\psi}_{s\bar{s}}^{m_j}(n, m, l) \phi_{nm}(\frac{\boldsymbol{k}_{\perp}}{\sqrt{x(1-x)}}) \chi_l(x)$$

2D harmonic oscillator Jacobi polynomial

 $2n + |m| + 1 \le N_{\max} \qquad l \le L_{\max}$ 

In this first work, we limit basis size to  $(N_{\max}, L_{\max}) = (1, 1)$  and  $(N_{\max}, L_{\max}) = (4, 1)$ 

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

The quark mass  $m_q$  and confining strength  $\kappa$  are slightly modified by fitting  $\rho(770)$  mass at  $N_{\text{max}} = L_{\text{max}} = 1$ , compared with original paper. [Qian, 2005.13806]

# Effective model of light mesons



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

		$H_{ m eff}^{(1,1)}$		$568487 \\ 0 \\ 25428 \\ 0 \\ 0$	$\begin{array}{c} 0 \\ 1700976 \\ 0 \\ -15767 \end{array}$	$\begin{array}{cccc} 25428 & 0 \\ 0 & -1576 \\ 568487 & 0 \\ 0 & 17009 \end{array}$		s in MeV
	n	m	l	s	$\overline{S}$	Direct encodi	ng Compact encoding	_
$\bigcirc$	0	0	0	1/2	-1/2	0001 angle	00 angle	
$\bigcirc$	0	0	0	-1/2	1/2	0010 angle	01 angle	
3	0	0	1	1/2	-1/2	0100 angle	10 angle	
(4)	0	0	1	-1/2	1/2	$ 1000\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.

# Encoding onto qubits

Setting up rules to map from physics problem to quantum computing problem

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

[Jordan and Wigner (1928)] [Seeley, 1208.5986]

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

[Kreshchuk, 2002.04016]

2. **Compact encoding**: 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 decomposition)

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

 $O(\log N) = O(n)$ 

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

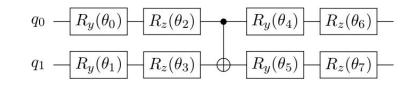
 $\operatorname{Tr}(P_j P_k) = 2^n \delta_{j,k} = N \delta_{j,k}$ 

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



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

- Barkoutsos [1805.04340] Romero [1701.02691] 1. Unitary coupled cluster (UCC) ansatz • motivated by coupled cluster methods  $\hat{U}(\vec{\theta}) = e^{\hat{T}(\vec{\theta}) - \hat{T}^{\dagger}(\vec{\theta})}, \quad \hat{T}(\vec{\theta}) = \hat{T}_1(\vec{\theta}) = \sum_{\substack{r \in \text{occ} \\ p \in \text{virt}}} \theta_p^r \hat{a}_p^{\dagger} \hat{a}_r$   $\hat{U}(\vec{\theta}) = e^{i \sum_{\alpha} c_{\alpha} P_{\alpha}}$   $\hat{U}(\vec{\theta}) = e^{i \sum_{\alpha} c_{\alpha} P_{\alpha}}$ UCC(Single) circuit for  $e^{i \theta_3^0 \hat{a}_3^{\dagger} \hat{a}_0}$
- 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



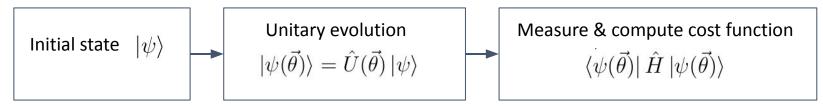
*EfficientSU2* ansatz with 1 repetition layer [Qiskit 0.32.1 library]

# **Optimization algorithms**

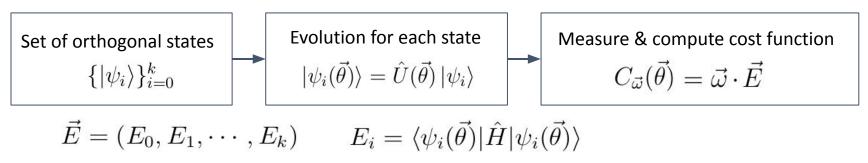


Variational Quantum Eigensolver (VQE) algorithm [Peruzzo, 1304.3061]

VQE finds the ground state

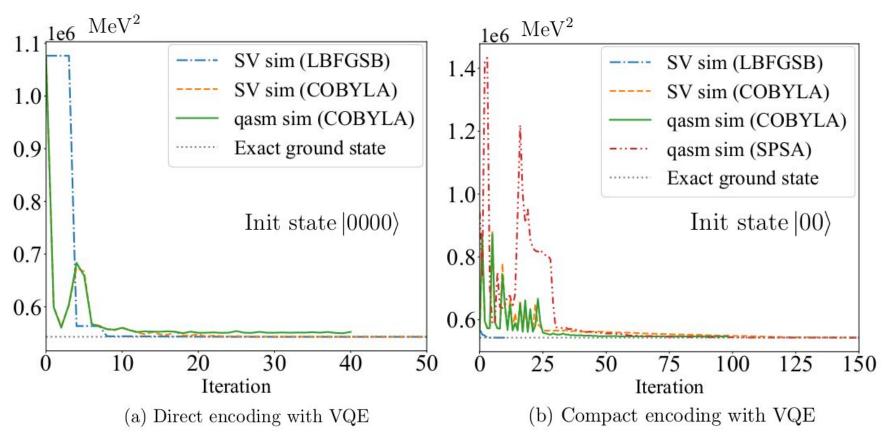


Subspace-search VQE (SSVQE) algorithm [Nakanishi, 1810.09434]
 In particular, Weighted SSVQE for finding up to k-th excited states



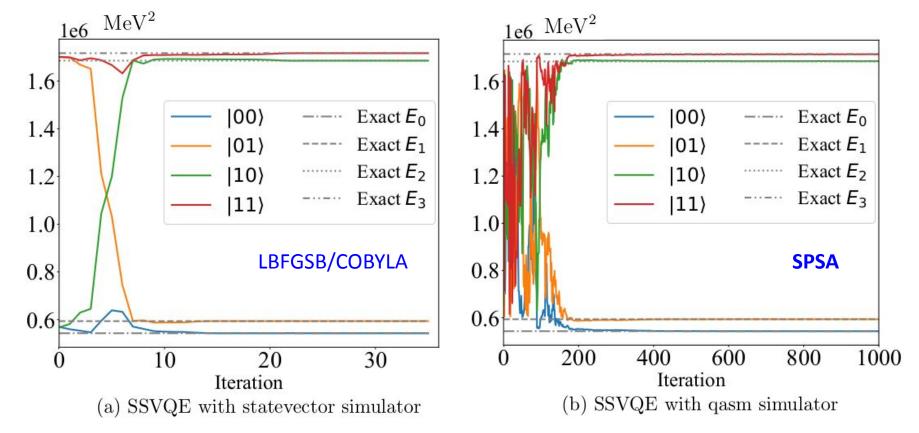
 $ec{\omega}$  is a strictly decreasing weight vector prioritizing lower-lying states

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



- All quantum simulated results agree with exact ground state energy.
- Ansatz: (a) UCCS ansatz, 50 gates (b) HE ansatz, 9 gates (1 repetition layer)
- Two IBM simulators are used: statevector (SV) simulator (exact simulation) and qasm simulator (8192 shots per measurement) [Qiskit 0.32.1 library]

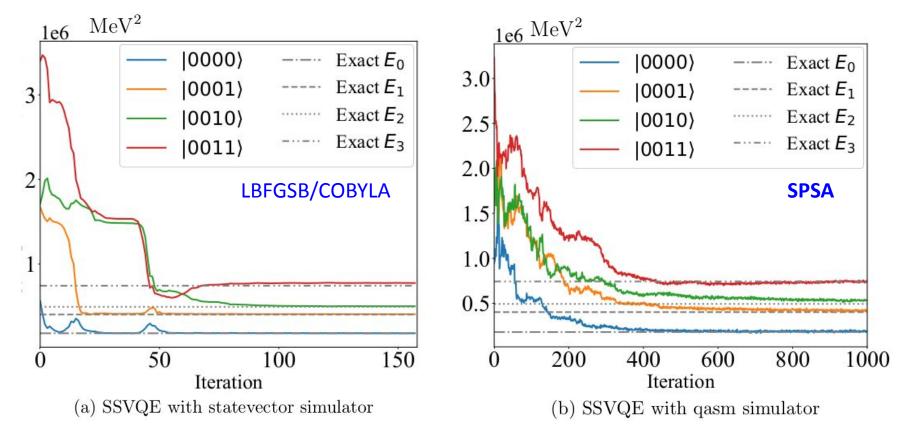
#### **Results: SSVQE spectrum** $(N_{\max}, L_{\max}) = (1, 1)$



- Both SV simulator (noise free) and qasm simulator (sampling noise) agree with exact classical spectrum.
- Both use HE ansatz (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: states emerge in accordance with the specified order of the cost function



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



- Low-lying spectrum, only look for lowest 4 states instead of 16
- Both SV simulator and qasm simulator do <u>NOT</u> completely agree with exact classical spectrum.
- Both use HE ansatz (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, we basically encode the basis representation of the LFWF on the qubits and evaluation of observables such as decay constants are straightforward:

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

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 ( $\pi$  and  $\rho$  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	$178.17 \pm 1.97$ $178.17 \pm 1.97$
4	1	$f_{\pi} \ f_{ ho}$	193.71 231.00	193.32 232.93	$\begin{array}{c} 194.28 \pm 15.49 \\ 225.72 \pm 13.44 \end{array}$

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

# Summary and outlook



We presented two promising quantum computing approaches, VQE and SSVQE, to find meson spectroscopy and observables (including decay constants) on the light front for the light meson systems.

Basis light-front quantization approach (BLFQ) works very 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 Logarithmic scaling (compact encoding)
  - Calculations on transition matrix element of an operator using SSVQE approach. Take advantage of **quantum superposition!**

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

$$\operatorname{Re}(A) = \langle \psi_{ij}^+ | U^{\dagger}(\vec{\theta}) \hat{A} U(\vec{\theta}) | \psi_{ij}^+ \rangle$$
  

$$- \frac{1}{2} (\langle \psi_i | U^{\dagger}(\vec{\theta}) \hat{A} U(\vec{\theta}) | \psi_i \rangle + \langle \psi_j | U^{\dagger}(\vec{\theta}) \hat{A} U(\vec{\theta}) | \psi_j \rangle)$$

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

Potential application: - EM radiative transition

18

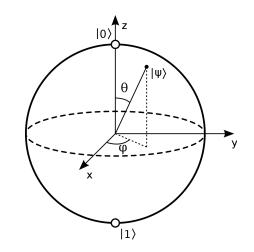
# Backup slides: Introduction to Quantum Computing

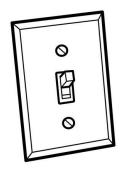
- Classical computers:
  - classical bit: 0, 1
  - implementation: electric voltage Low, High
  - classical gates: AND, OR, NOT, Bitwise logic gates
  - Deterministic nature

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

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

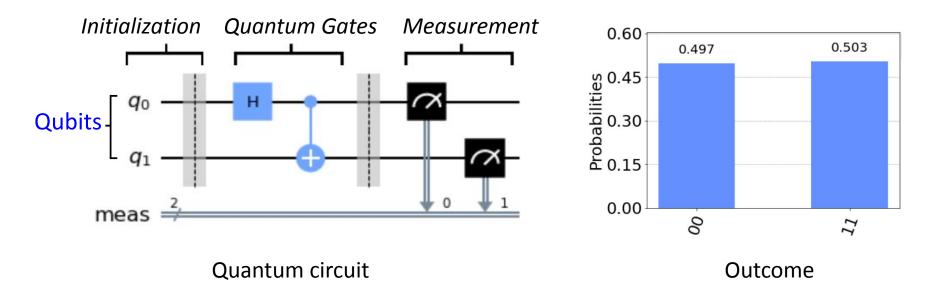
- quantum gates: unitary operators
- States only collapse when measured
- <u>superposition</u>
- Can theoretically solve problems classical computers cannot solve







# Backup slides: Quantum circuit crash course



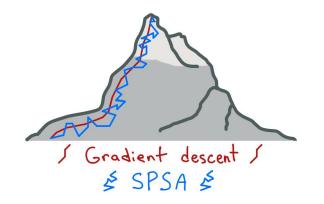
- Each horizontal line represents the evolution of a qubit (from left to right)
- Each measurement collapses the wave function and we obtain either 0 or 1 in the computation basis
- In practice, measurements are statistical outcomes by running the same circuit repeatedly for thousands of times (or shots)

# Backup slides: 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

# Backup slides: Parton distribution functions



We can also use quantum simulators to measure parton distribution functions (PDFs), which is the probability of finding a particle with longitudinal momentum fraction x under some factorization scale related to experimental conditions,

$$q(x;\mu) = \frac{1}{x(1-x)} \sum_{s\bar{s}} \int \frac{\mathrm{d}^2 \mathbf{k}_{\perp}}{2(2\pi)^3} |\psi_{s\bar{s}}^{(m_j=0)}(x,\mathbf{k}_{\perp})|^2$$

$$\equiv \frac{1}{4\pi} \sum_{s\bar{s}} \sum_{nm} \sum_{l\bar{l}} \tilde{\psi}_{s\bar{s}}^{*(m_j=0)}(n,m,\bar{l}) \tilde{\psi}_{s\bar{s}}^{(m_j=0)}(n,m,l) \chi_l(x) \chi_{\bar{l}}(x)$$
[Li, 1704.06968]

Using projection operators, we can compute the PDF on quantum computers as well. Note that the PDF operator on qubits will be dependent on *x*.

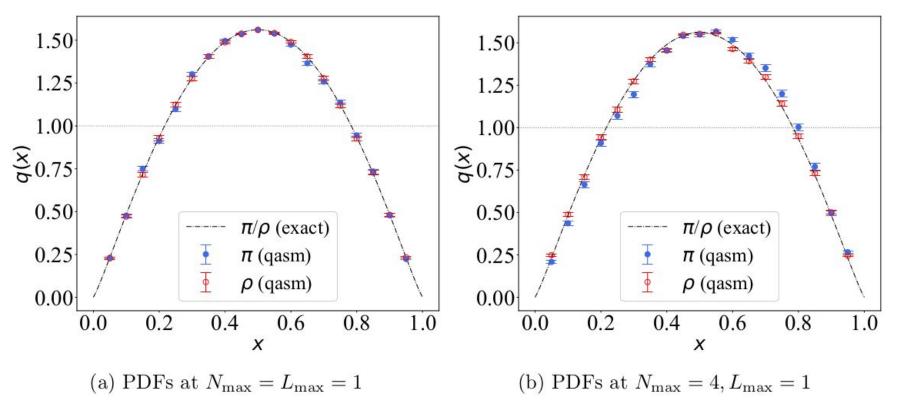
$$q(x) = \sum_{s\bar{s}} \sum_{nm} \sum_{l\bar{l}} \langle \psi(\vec{\theta}) | \hat{O}_{pdf}(x) | \psi(\vec{\theta}) \rangle$$

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

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

# Backup slides: Parton distribution functions





- In both basis truncations, the PDFs for lowest two states are comparable due to the lack of longitudinal excitations. Note: SV and exact results agree with each other (not shown).
- For  $(N_{\max}, L_{\max}) = (1, 1)$ , the qasm agree with the exact calculations.
- For  $(N_{\text{max}}, L_{\text{max}}) = (4, 1)$ , the PDF is rescaled due to lack of normality of the PDF (or LFWF on qubits) as the SSVQE evolution is sensitive to sample noise at this cutoff.



#### Backup slides: Detailed Statistics of VQE results

Simulator	Encoding	Optimizer	Ground state energy $(MeV^2)$	Iterations
	Direct	LBFGSB	543059~(0%)	60
SV	Direct	COBYLA	543059~(0%)	90
	Compact	LBFGSB	543059~(0%)	11
	Compact	COBYLA	543059~(0%)	344
	Direct	COBYLA	$552344 \pm 996 \ (1.53\%)$	41
qasm	Direct	SPSA	$545767 \pm 152 \ (0.47\%)$	1051
1	Compact	COBYLA	$547405 \pm 211 (0.76\%)$	99
	Compact	SPSA	$543065 \pm 6  (0\%)$	1551
Exact solution	-	-	543059	



#### Backup slides: Detailed Statistics of SSVQE results

$N_{ m max}$	$L_{\max}$	State	Exact energy $(MeV^2)$	$SV sim (MeV^2)$	qasm sim $(MeV^2)$
		$ 00\rangle$	543059	543059 (0%)	$543059 \pm 0 \ (0\%)$
1	1	$ 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%)	$745422\pm 6503~(2.88\%)$



#### Backup slides: Hamiltonian on qubits

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

 $H_{\rm compact}^{(4,1)} = 1868696\,IIII - 623614\,IIIZ + 518799\,IIXI + 44344\,IIXZ$ -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,



## Backup slides: Basis mapping for $(N_{\max}, L_{\max}) = (4, 1)$

	n	m	l	s	$\bar{s}$	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 angle
(4)	0	0	1	-1/2	1/2	$ 0011\rangle$
(5)	0	1	0	-1/2	-1/2	$ 0100\rangle$
$\bigcirc$	0	1	1	-1/2	-1/2	0101 angle
$\overline{7}$	0	-1	0	1/2	1/2	$ 0110\rangle$
8	0	-1	1	1/2	1/2	$ 0111\rangle$
9	1	0	0	1/2	-1/2	$ 1000\rangle$
(10)	1	0	0	-1/2	1/2	$ 1001\rangle$
11	1	0	1	1/2	-1/2	$ 1010\rangle$
(12)	1	0	1	-1/2	1/2	$ 1011\rangle$
(13)	1	1	0	-1/2	-1/2	$ 1100\rangle$
(14)	1	1	1	-1/2	-1/2	1101 angle
(15)	1	-1	0	1/2	1/2	$ 1110\rangle$
$\boxed{16}$	1	-1	1	1/2	1/2	$ 1111\rangle$