# Simulating Subatomic Physics on a Quantum Frequency Processor

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1 / 42

#### How Did This Work Come About?



PRL 120, 030502 (2018)



PRL 120, 210501 (2018)

#### Simulations of Subatomic Many-Body Physics on a Quantum Frequency Processor

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arXiv:1810.03959



2 / 42

## Quantum Computing for Subatomic Physics Programme

- Ab initio calculations of nucleon and nuclear matter properties from lattice quantum chromodynamics (QCD)
- Effective field theory (EFT) description of nulcei
- Explain astrophysical events at extreme nucleon densities





3 / 42

#### Nuclear EFT Systems of Interest



 $\ensuremath{\mathbf{Q}}\xspace$ : Compute the binding energy from an EFT Hamiltonian

$$V \rightarrow \int d\mathbf{r} \Psi^{\dagger}(\mathbf{r}) V_{1} \Psi(\mathbf{r}) + \int d\mathbf{r} d\mathbf{r}' \Psi^{\dagger}(\mathbf{r}) \Psi^{\dagger}(\mathbf{r}') V_{2} \Psi(\mathbf{r}) \Psi(\mathbf{r}')$$

$$+ \cdots$$

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#### From Lattice QFT to EFT: The Schwinger Model

- The Schwinger model is QED in one space and one time dimension
- The Lagrangian for the continuum model:

$$\mathcal{L} = \overline{\psi} (i \not\!\!D - m) \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}$$

- spatially discretized with the Kogut-Susskind (staggered) action
- mapped onto qubits using the JW transformation



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5 / 42

# How Can Near-Term Quantum Computers Help in Scientific Applications?

- Calculating N-qubit observables on a classical computer is a problem for  $N \ge 50$ 
  - $|\psi
    angle$  is an N-qubit state,  $\hat{O}$  is an N-qubit observable
  - Representing  $|\psi\rangle$  needs  $O(2^N)$  classical bits
  - $\langle \psi | \hat{O} | \psi \rangle$  reduces to a matrix-vector multiplication on a classical computer with  $O(2^{2N})$  operations
- Calculating N-qubit observables on a quantum computer requires N qubits
  - Prepare the N-qubit state  $|\psi
    angle$  M times
  - Measure  $\hat{O}$  each time  $|\psi
    angle$  is prepared
  - Compute the average  $pprox \langle \psi | \hat{O} | \psi 
    angle$

6 / 42

Particularly of interest in scientific apps is a ground-state energy of *N*-body systems.

Algorithm 1 Variational Quantum Eigensolver Algorithm

initialize variational parameter  $\boldsymbol{\theta}_0 = \{ \theta_0^1, \cdots, \theta_0^M \}$ 

```
while \operatorname{grad}(\langle \Psi(\boldsymbol{\theta}_{\boldsymbol{i}}) | H | \Psi(\boldsymbol{\theta}_{\boldsymbol{i}}) \rangle) \geq \epsilon do
```

quantum compute  $\langle \Psi(m{ heta}_i)|H|\Psi(m{ heta}_i)
angle$ 

classical update  $\theta_{i+1}$ return min  $\langle \Psi(\theta) | H | \Psi(\theta) \rangle$ 



## Introducing the Hardware: Quantum Frequency Processor





Optica 5 , 1455-1460 (2018)

#### Mapping Subatomic Problems onto a QFP

- Start with a N-body second-quantized Hamiltonian  $H_{SQ}$
- Project  $H_{SQ}$  onto eigenstates of operators that represent good quantum numbers (e.g., parity, momentum, total spin) for the system of interest. ( $\tilde{\mathcal{H}}_{SQ} = \bigoplus_i \mathcal{H}_i$ )
- $\mathcal{H}_i$ s can now be interpreted as single-particle Hamiltonians and mapped onto a frequency bin multiport device

$$\mathcal{H}_{QFP}^{i} = \sum_{k=0}^{d-1} h_{kk} c_{k}^{\dagger} c_{k} + \sum_{\substack{k,l=0\\k < l}}^{d-1} [h_{kl} c_{k}^{\dagger} c_{l} + h_{kl}^{*} c_{l}^{\dagger} c_{k}]$$

• Single particle (photon) variation wavefunction

1/24/2019

9 / 42

#### VQE: Single Photon vs Coherent State

- We use QFP to compute  $H_{k,l} = \langle \Psi | h_{kl} c_k^{\dagger} c_l + h_{kl}^* c_l^{\dagger} c_k | \Psi \rangle$  for all k, l
- For  $H_{k,l}$  computation single-photon state

$$|\Psi\rangle = \cos\phi |10\cdots0\rangle - \frac{\sin\phi}{\phi} \sum_{k=1}^{d-1} \theta_k |0\cdots1_k\cdots0\rangle$$

and

$$|\Psi_{\rm comb}\rangle = |\alpha\cos\phi\rangle \otimes \left|\alpha e^{i\pi}\frac{\theta_1\sin\phi}{\phi}\right\rangle \otimes \cdots \otimes \left|\alpha e^{i\pi}\frac{\theta_{d-1}\sin\phi}{\phi}\right\rangle$$

are equivalent



10 / 42

#### Light Nuclei Simulations



All-optical quantum frequency processor



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#### EFT for the Schwinger 4-lattice-site Problem



Effective 2-body potential between heavy charges in the 4-lattice-site Schwinger model

[arXiv:1810.03959]



12 / 42

Natalie Klco, Martin Savage, Alessandro Roggero, Kody Law, Ajay Jasra, Mikel Sanz, Lucas Lamata, Enrique Solano, Ryan Bennink, Travis Humble, Thomas Maier, Alex McCaskey, Shirley Moore, Nicholas Peters, Gaute Hagen, Gustav Jansen, David Dean, Raphael Pooser, Eugene Dumitrescu, Hsuan-Hao Lu, Joe Lukens, Aaina Bansal, Andreas Ekström, Andrew M Weiner, Titus Morris, Thomas Papenbrock.

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13 / 42

#### Thank You! Questions?



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/24/2019 14

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https://jobs.ornl.gov/job/Oak-Ridge-Research-Scientist-in-Quantum-Information-Science-TN-37831/520601100/ Multiple Postdoc Positions



image https://www.visitsmokies.org



15 / 42

- Typically an observable of interest is energy
- Take a Hamiltonian H = T + V and write it in a second-quantized form using field operators Ψ(r), Ψ<sup>†</sup>(r)
- The kinetic energy  ${\cal T} 
  ightarrow \int d{f r} \Psi^\dagger({f r}) {\cal T} \Psi({f r})$
- The potential energy

$$V \rightarrow \int d\mathbf{r} \Psi^{\dagger}(\mathbf{r}) V_{1} \Psi(\mathbf{r}) + \int d\mathbf{r} d\mathbf{r}' \Psi^{\dagger}(\mathbf{r}) \Psi^{\dagger}(\mathbf{r}') V_{2} \Psi(\mathbf{r}) \Psi(\mathbf{r}') + \cdots$$





16 / 42

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- Discretize field operators  $\Psi(\mathbf{r}) = \sum_{n=0}^{N} \psi_n(\mathbf{r})c_n$ ,  $c_n$  is a single-particle annihilation operator
- Re-write *H* in terms of  $c_n$  and  $c_n^{\dagger}$ :

$$H = \sum_{n,m} (T_{nm} + V_{nm})c_n^{\dagger}c_m + \sum_{n,m,k,l} V_{nmkl}c_n^{\dagger}c_m^{\dagger}c_kc_l + \cdots$$

• Map  $c_n$  and  $c_n^{\dagger}$  onto Pauli X, Y, Z operators (qubits = spin 1/2!).





17 / 42

- We will need to prep an *N*-qubit state  $|\psi(\theta_1, \cdots \theta_N)\rangle$  to evaluate  $\langle \psi(\theta_1, \cdots \theta_N) | H | \psi(\theta_1, \cdots \theta_N) \rangle$
- $|\psi(\theta_1,\cdots,\theta_N)\rangle = U(\theta_1,\cdots,\theta_N)|0,\cdots,0\rangle$
- We will need to decompose U(θ<sub>1</sub>, · · · θ<sub>N</sub>) into a sequence of one- and two-qubit operations that quantum hardware can implement
- Optimize the decomposition to minimize the use of precious two-qubit gates





18 / 42

1/24/2019

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Domain science Hamiltonian Discretize and map to gubits Generate quantum circuit for the problem Circuit optimization Hardware execution Post processing



19 / 42

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• Existing quantum hardware is noisy. Simulation results require post processing to remove systematic effects of noise



- The deuteron is the lightest nucleus consisting of a neutron and a proton
- Binding energy  $E_B = -2.2 \text{ MeV}$  (measured)
- Use quantum computer to calculate the binding energy



20 / 42

#### The Deuteron: Hamiltonian Model

- The Deuteron is a two-body system with the Hamiltonian in the center-of-mass frame H = T + V
- The kinetic energy  $T = \frac{p^2}{2\mu}$
- The potential V(r) is specially chosen to reproduce deuteron's binding energy
- We want to use quantum computers to calculate the smallest eigenvalue of *H* (binding energy)
- More precisely, we would like to compute  $\langle \Psi | H | \Psi \rangle$  for a class of  $|\Psi \rangle$
- Minimizing  $\langle \Psi | H | \Psi \rangle$  over all  $| \Psi \rangle$  will give an estimate of the binding energy



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#### The Deuteron: Second-Quantized Hamiltonian

- First we need to rewrite  $H = \frac{p^2}{2\mu} + V(r)$  in the second-quantized form
- We use harmonic oscillator basis (Fock states |n>, n = 0, · · · , N and single particle creation (annihilation) operators c<sup>†</sup><sub>n</sub>(c<sub>n</sub>))

• In this basis 
$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|H|n 
angle c_{n'}^\dagger c_n$$

We evaluate matrix elements in the Fock basis:

$$\langle n' | V(r) | n \rangle = V_0 \delta_n^0 \delta_n^{n'} \langle n' | \frac{p^2}{2\mu} | n \rangle = \frac{\hbar \omega}{2} \bigg[ (2n+3/2) \delta_n^{n'} - \sqrt{n(n+1/2)} \delta_n^{n'+1} - \sqrt{(n+1)(n+3/2)} \delta_n^{n'-1} \bigg]$$



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22 / 42

#### The Deuteron: Mapping to Qubits

• We use Jordan-Wigner transform

$$c_n^\dagger 
ightarrow rac{1}{2} \left[ \prod_{j=0}^{n-1} - Z_j 
ight] (X_n - iY_n); c_n 
ightarrow rac{1}{2} \left[ \prod_{j=0}^{n-1} - Z_j 
ight] (X_n + iY_n)$$

- A spin up | ↑⟩ (down | ↓⟩) state of the qubit n corresponds to zero (one) deuteron in the state |n⟩.
- Hamiltonians for N = 2, 3:

$$\begin{aligned} H_2 &= 5.906709I + 0.218291Z_0 - 6.125Z_1 \\ &- 2.143304 \left( X_0 X_1 + Y_0 Y_1 \right), \\ H_3 &= H_2 + 9.625 (I - Z_2) \\ &- 3.913119 \left( X_1 X_2 + Y_1 Y_2 \right) \end{aligned}$$



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1/24/2019

23 / 42

## The Deuteron: Computing the Binding Energy

- Compute the binding energy  $E_N$  using VQE and the Unitary Coupled-Cluster ansatz for all N up to  $N_{max}$
- Extrapolate to the continuum  $E_{\infty}$  by using  $E_1, \cdots, E_{N_{max}}$
- For the extrapolation to the infinite space we employ the harmonic-oscillator variant of Lüscher's formula for finite-size corrections to the ground-state energy:

$$E_{N} = -\frac{\hbar^{2}k^{2}}{2m} \left(1 - 2\frac{\gamma^{2}}{k}e^{-2kL} - 4\frac{\gamma^{4}L}{k}e^{-4kL}\right) \\ + \frac{\hbar^{2}k\gamma^{2}}{m} \left(1 - \frac{\gamma^{2}}{k} - \frac{\gamma^{4}}{4k^{2}} + 2w_{2}k\gamma^{4}\right)e^{-4kL},$$

L = L(N) is the effective hard-wall radius for the finite basis of dimension N, k is the bound-state momentum,  $\gamma$  the asymptotic normalization coefficient, and  $w_2$  an effective range parameter.

24 / 42

#### The Deuteron: VQE and UCC Quantum Circuits

• Unitary Coupled-Cluster ansatz for N = 2 (two qubits):

$$|\Psi_{UCC}\rangle \equiv e^{\theta \left(c_0^{\dagger}c_1 - c_1^{\dagger}c_0\right)} |\downarrow\uparrow\rangle = \cos\theta |\downarrow\uparrow\rangle - \sin\theta |\uparrow\downarrow\rangle$$

• Unitary Coupled-Cluster ansatz for N = 3 (three qubits):

$$\begin{array}{ll} |\Psi_{UCC}\rangle & \equiv & e^{\sum\limits_{i=1}^{N-1} \theta_i \left(c_0^{\dagger} c_i - c_i^{\dagger} c_0\right)} |\downarrow\uparrow\uparrow\rangle = \cos(\theta_1) |\downarrow\uparrow\uparrow\rangle \\ & - & \sin(\theta_1)\cos(\theta_2) |\uparrow\downarrow\uparrow\rangle - \sin(\theta_1)\sin(\theta_2) |\uparrow\uparrow\downarrow\rangle \end{array}$$

Quantum circuits:







25 / 42

#### The Deuteron: VQE Results N = 2



• Quantum circuit  $|\uparrow\rangle$  X + $|\uparrow\rangle$   $e^{i\theta Y}$  +



- $H_2 = 5.906709I$ 
  - $+ 0.218291Z_0 6.125Z_1$
  - $-2.143304(X_0X_1+Y_0Y_1)$





26 / 42

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## The Deuteron: VQE Experimental Results N = 3



## The Deuteron: Extrapolating to Zero-Noise Results N = 3

• Two-qubit CNOT gates are imperfect, with error rate e



• If e is small, inserting noisy 1 gates into the variational circuit will result in the energy change

$$H(r) = H(0) - reH(0)$$







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#### The Deuteron: VQE Results N = 3



1/24/2019 29 / 42

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#### The Deuteron: Putting It All Together

The exact binding energy of the deuteron  $E_{\infty} = -2.22$  MeV.

<i>E</i> from exact diagonalization				
N	E <sub>N</sub>	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	-1.749	-2.39	-2.19	
3	-2.046	-2.33	-2.20	-2.21
E from quantum computing				
N	E <sub>N</sub>	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	-1.74(3)	-2.38(4)	-2.18(3)	
3	-2.08(3)	-2.35(2)	-2.21(3)	-2.28(3)

$$E_{N} = -\frac{\hbar^{2}k^{2}}{2m} \left(1 - 2\frac{\gamma^{2}}{k}e^{-2kL} - 4\frac{\gamma^{4}L}{k}e^{-4kL}\right) \\ + \frac{\hbar^{2}k\gamma^{2}}{m} \left(1 - \frac{\gamma^{2}}{k} - \frac{\gamma^{4}}{4k^{2}} + 2w_{2}k\gamma^{4}\right)e^{-4kL}$$

[PRL 120 210501; arXiv:1801.03897]

30 / 42

### Lattice Quantum Field Theories on a Quantum Computer





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1/24/2019 31 / 42

- $\bullet\,$  The Schwinger model describes quantum electrodynamics in one space and one time dimension, 1+1
- Key features: confinement and spontaneous breaking of chiral symmetry (QCD-like)
- The vacuum of the theory enjoys a non-zero condensate,  $\langle \psi \overline{\psi} 
  angle$
- The Lagrangian for the continuum model:

$$\mathcal{L} = \overline{\psi} (i \not\!\!D - m) \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}$$



32 / 42

#### The Schwinger model can be

- spatially discretized with the Kogut-Susskind (staggered) action
- mapped onto a (re-scaled) Hamiltonian density using the Jordan-Wigner transformation
- gauge-fixed by setting the temporal component of the gauge field to zero ( $A_0 = 0$ ) on  $N_Q/2$  spatial sites

$$\hat{H} = x \sum_{n=0}^{N_Q-1} \left( \sigma_n^+ L_n^- \sigma_{n+1}^- + \sigma_{n+1}^+ L_n^+ \sigma_n^- \right) + \sum_{n=0}^{N_Q-1} \left( l_n^2 + \frac{\mu}{2} (-)^n Z_n \right)$$

[we will use x = 0.6 and  $\mu = 0.1$  throughout this presentation]



33 / 42



Qubit and electric flux link structure of the two-spatial-site lattice Schwinger model Naïve qubit count

- Two qubits are sufficient to describe the fermion occupation of a single spatial lattice site, one for the e<sup>-</sup> and one the e<sup>+</sup>.
- We cut off the range of values of each  $l_n$  ( $|l_n| \le 1$ ), thus two qubits per flux link
- Total qubit # to simulate two-lattice site dynamics 2+2+4\*2 = 12



Natural symmetries of the Schwinger 1 + 1 model:

- Local Abelian gauge symmetry U(1)
- Parity transformation  $\hat{P}_a$  (reflection of the system through axes that preserves the structure of the Wigner-Jordan representation of the fermionic fields)
- Charge conjugation  $\hat{C}_i$  transforms particles into antiparticles and vice versa, and the direction of the electric field reverses as a result (an additional directional shift by one lattice site is necessary)
- *Translation* symmetry (natural on a lattice with PBC) leads to the momentum conservations



35 / 42

### The Schwinger Model: Parity Symmetry Examples

Parity transform for the one-spatial-site lattice Schwinger mode:



Parity transform for the two-spatial-site lattice Schwinger model:



13 physical states satisfy Gauss's law in the charge Q = 0 sector:

$$\begin{split} |\phi_1\rangle &= |\cdots\rangle |0000\rangle \\ |\phi_2\rangle &= |\cdots\rangle |1111\rangle \\ |\phi_3\rangle &= |\cdots\rangle |-1-1-1-1\rangle \\ |\phi_4\rangle &= |e^-e^+ \cdots\rangle |-1000\rangle \\ |\phi_5\rangle &= |\cdot e^-e^+\rangle |00-10\rangle \\ |\phi_6\rangle &= |e^-e^+ \cdots\rangle |0111\rangle \\ |\phi_7\rangle &= |\cdot e^-e^+\rangle |1101\rangle \end{split}$$

$$\begin{aligned} |\phi_{8}\rangle &= |e^{-}e^{+}e^{-}e^{+}\rangle| - 10 - 10\rangle \\ |\phi_{9}\rangle &= |e^{-}e^{+}e^{-}e^{+}\rangle|0101\rangle \\ |\phi_{10}\rangle &= |e^{-}\cdot\cdot e^{+}\rangle| - 1 - 1 - 10\rangle \\ |\phi_{11}\rangle &= |e^{-}\cdot\cdot e^{+}\rangle|0001\rangle \\ |\phi_{12}\rangle &= |\cdot e^{+}e^{-}\cdot\rangle|0100\rangle \\ |\phi_{13}\rangle &= |\cdot e^{+}e^{-}\cdot\rangle| - 10 - 1 - 1\rangle \end{aligned}$$



37 / 42

Sectors of definite momentum, **k**, constrained to satisfy  $\mathbf{k} = \pi n$  with  $n = 0, \pm 1$ :

$$\begin{aligned} |\psi_{1}\rangle_{\mathbf{k}=\mathbf{0}} &= |\phi_{1}\rangle \\ |\psi_{2}\rangle_{\mathbf{k}=\mathbf{0}} &= |\phi_{2}\rangle \\ |\psi_{3}\rangle_{\mathbf{k}=\mathbf{0}} &= |\phi_{3}\rangle \\ |\psi_{4}\rangle_{\mathbf{k}=\mathbf{0}} &= \frac{1}{\sqrt{2}} \left[ |\phi_{4}\rangle + |\phi_{5}\rangle \right] \\ |\psi_{5}\rangle_{\mathbf{k}=\mathbf{0}} &= \frac{1}{\sqrt{2}} \left[ |\phi_{6}\rangle + |\phi_{7}\rangle \right] \end{aligned} \qquad \begin{aligned} |\psi_{6}\rangle_{\mathbf{k}=\mathbf{0}} &= |\phi_{8}\rangle \\ |\psi_{7}\rangle_{\mathbf{k}=\mathbf{0}} &= |\phi_{9}\rangle \\ |\psi_{8}\rangle_{\mathbf{k}=\mathbf{0}} &= \frac{1}{\sqrt{2}} \left[ |\phi_{10}\rangle + |\phi_{13}\rangle \right] \\ |\psi_{9}\rangle_{\mathbf{k}=\mathbf{0}} &= \frac{1}{\sqrt{2}} \left[ |\phi_{11}\rangle + |\phi_{12}\rangle \right] \end{aligned}$$



# The Schwinger Model: Gauge, Momentum, Charge & Parity

Sectors of definite momentum,  $\mathbf{k} = \mathbf{0}$ ,  $\hat{C}\hat{P} = \pm 1$ , and charge Q = 0 :

$$\begin{aligned} |\chi_1\rangle_{\mathbf{k}=\mathbf{0},+} &= |\psi_1\rangle \\ |\chi_2\rangle_{\mathbf{k}=\mathbf{0},+} &= \frac{1}{\sqrt{2}} \left[ |\psi_4\rangle + |\psi_9\rangle \right] \\ |\chi_3\rangle_{\mathbf{k}=\mathbf{0},+} &= \frac{1}{\sqrt{2}} \left[ |\psi_6\rangle + |\psi_7\rangle \right] \end{aligned} \qquad \begin{aligned} |\chi_4\rangle_{\mathbf{k}=\mathbf{0},+} &= \frac{1}{\sqrt{2}} \left[ |\psi_5\rangle + |\psi_8\rangle \right] \\ |\chi_5\rangle_{\mathbf{k}=\mathbf{0},+} &= \frac{1}{\sqrt{2}} \left[ |\psi_2\rangle + |\psi_3\rangle \right] \end{aligned}$$

$$\begin{aligned} |\chi_1\rangle_{\mathbf{k}=\mathbf{0},-} &= \frac{1}{\sqrt{2}} \left[ |\psi_4\rangle - |\psi_9\rangle \right] & |\chi_3\rangle_{\mathbf{k}=\mathbf{0},-} &= \frac{1}{\sqrt{2}} \left[ |\psi_5\rangle - |\psi_8\rangle \right] \\ |\chi_2\rangle_{\mathbf{k}=\mathbf{0},-} &= \frac{1}{\sqrt{2}} \left[ |\psi_6\rangle - |\psi_7\rangle \right] & |\chi_4\rangle_{\mathbf{k}=\mathbf{0},-} &= \frac{1}{\sqrt{2}} \left[ |\psi_2\rangle - |\underbrace{\psi_8}_{\mathrm{Nutual Laboratory}} \right] \end{aligned}$$

#### The Schwinger Model: Recapping the Symmetries

• By using the eigenstates of the Momentum, Charge, Parity operators we have preconditioned the Schwinger Hamiltonian *H*,

$$H \equiv \bigoplus_{i=\{\mathbf{k}, CP\}} H_i$$

• The non-trivial dynamics happens in two subspaces:

$$H_{\mathbf{k}=\mathbf{0},+} = \begin{pmatrix} -2\mu & 2x & 0 & 0 & 0 \\ 2x & 1 & \sqrt{2}x & 0 & 0 \\ 0 & \sqrt{2}x & 2+2\mu & \sqrt{2}x & 0 \\ 0 & 0 & \sqrt{2}x & 3 & \sqrt{2}x \\ 0 & 0 & 0 & \sqrt{2}x & 4-2\mu \end{pmatrix}$$

$$H_{\mathbf{k}=\mathbf{0},-} = \begin{pmatrix} 1 & \sqrt{2}x & 0 & 0 \\ \sqrt{2}x & 2+2\mu & -\sqrt{2}x & 0 \\ 0 & -\sqrt{2}x & 3 & \sqrt{2}x \\ 0 & 0 & \sqrt{2}x & 4-2\mu \end{pmatrix}$$

• Reduced # of qubits from **12** to  $\leq$ **3**! Pavel Lougovski (ORNL)

- Working with the **k** = **0** CP = +1 sector, we are interested in the dynamics of the unoccupied state  $|\chi_1\rangle_{\mathbf{k}=\mathbf{0},+}$
- Trotterization  $e^{-iHt} 
  ightarrow \lim_{N 
  ightarrow \infty} \left( \prod_{j} e^{-iH_{j}\delta t} \right)^{N}$
- Exact SU(4) dynamics  $e^{-iHt} = K^T CK$  where  $C \approx e^{-iXX} e^{-iYY} e^{-iZZ}$  $K \in SU(2) \otimes SU(2)$



41 / 42

#### The Schwinger Model: Simulation Results IBM QX2



#### [PRA 98 032331; arXiv:1803.03326]



42 / 42