# Quantum Computing: a future perspective for scientific computing

**Quantum Computing** 

Karl Jansen Cairns, The XVIth Quark Confinement and the Hadron Spectrum Conference, 19.8.2024



### **Overview**

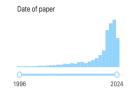


- > Short intro to quantum computing
- Application to QED in 1+1, 2+1 and 3+1 dimensions
- > Non-abelian gauge theories
- > Real time dynamics
- > PDFs
- > Conclusion

### **Statistics**

### According to inspire, 4.8.24:

> find t qubits: since 2020 1,327 papers

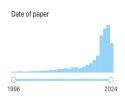


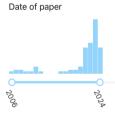
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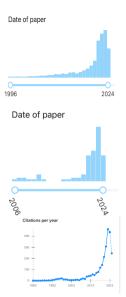
### **Statistics**

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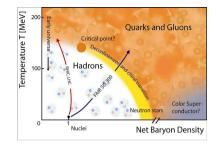
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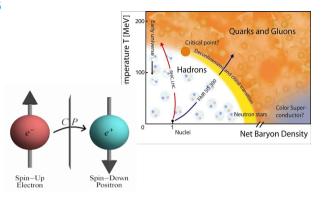
> Feynman's "Simulating physics with computers",  $\rightarrow$  2,521 citations



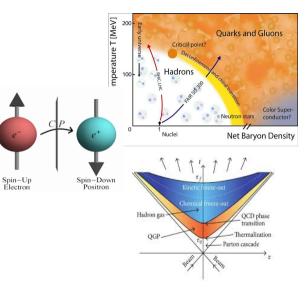
- > Non-zero chemical potential
  - early universe
  - neutron stars, new phases, ...



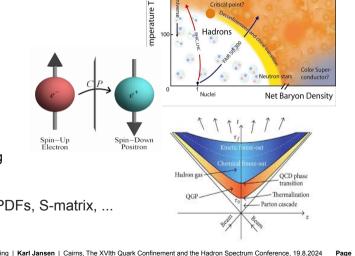
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- > Minkowski time observables, PDFs, S-matrix, ...

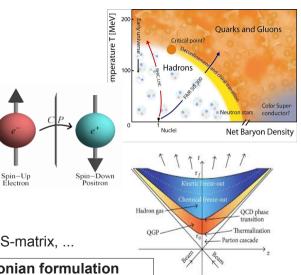


**Ouarks and Gluons** 

[MeV]

- Non-zero chemical potential >
  - early universe
  - neutron stars, new phases, ...
- **Topological terms** 
  - **CP-violation**
  - topological materials, ...
- Real time dynamics
  - heavy ion collisions, scattering
  - quenches....
- Minkowski time observables, PDFs, S-matrix, ...

⇒ Hamiltonian formulation



### A problem with Hamiltonian approach



• determine wave function  $|\Psi>$ 

 $|\Psi> = \sum_{i_1, i_2, \cdots, i_N} C_{i_1, i_2, \cdots, i_N} |i_1 i_2 \cdots i_N>$ 

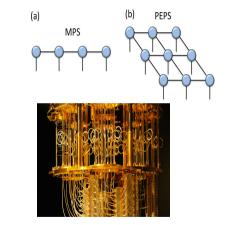
 $C_{i_1,i_2,\cdots,i_N}$  coefficient matrix with  $2^N$  entries

 $\rightarrow$  problem scales exponentially

# Two solutions for Hamiltonian approach

- > Tensor Networks
  - gapped, local Hamiltonians
    - $\rightarrow$  area law
    - $\rightarrow$  very fast (exponential) convergence
  - costly: entanglement
    - ightarrow phase transitions, (long) real time evolution
- > Quantum Computing
  - conceptually clean path
  - noise, low number of qubits, ...





### > Here: focus on quantum computing Quantum Field Theories

••

### Quantum computer: from the outside



### some qubit players

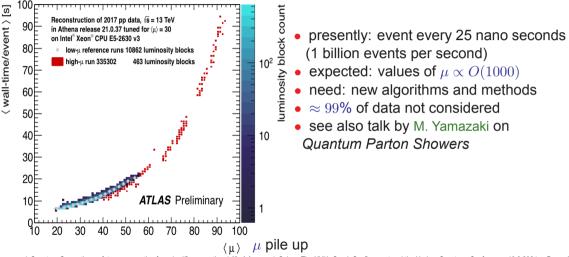
- > Superconducting
  - fast, high fidelity, needs cooling
- > Trapped ions
  - very high fidelity, no extreme cooling, slow
- > Photonics
  - extremely fast, no cooling, noisy
- > Neutral atoms
  - long coherence times, no cooling, ultrahigh vacuum
- > Silicon Spin/Quantum dots
  - fast and good fidelity, very much in development
- > analoque computing, adiabatic computing, ...

# Quantum computer: from the inside (superconducting)



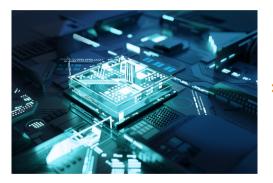
- Shielded to 50,000 times less than Earth's magnetic field
- In a high vacuum: pressure is 10 billion times lower than atmospheric pressure
- Cooled 180 times colder than interstellar space (0.015 Kelvin)
   → prevent quantum noise
- IBMQ: 433 qubits 2022, >1000 qubits 2023, >4000 qubits 2024  $\rightarrow$  10K to 100K error corrected, parallelized
- Google promise: 1.000.000 qubits 2030, 1000 qubits error corrected

### **Computing challenge for High-Lumi LHC**



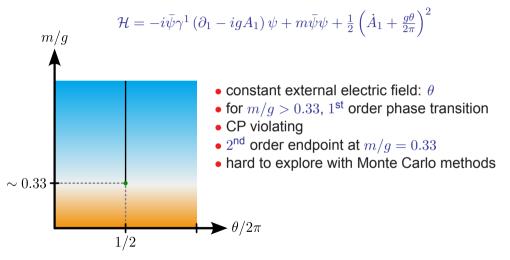
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### **Overview**



### Application to QED in 1+1, 2+1 and 3+1 dimensions

### Schwinger model in the continuum and phase diagram



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### Schwinger model on the lattice: Wilson fermions

(Takis Angelides, Arianna Crippa, Lena Funcke, Karl Jansen, Stefan Kühn, Pranay Naredi, Ivano Tavernelli, Derek Wang, arxiv:2312.12831)

> Wilson Hamiltonian

$$\begin{split} H_W &= \sum_{n=0}^{N-2} \left( \bar{\phi}_n \left( \frac{1+i\gamma^1}{2a} \right) U_n \phi_{n+1} + \text{ h.c. } \right) \\ &+ \sum_{n=0}^{N-1} \left( m_{\text{lat}} + \frac{1}{a} \right) \bar{\phi}_n \phi_n + \sum_{n=0}^{N-2} \frac{ag^2}{2} \left( L_n + l_0 \right)^2, \quad U_\mu = e^{iagA_\mu} \end{split}$$

> mass  $m_{\mathsf{lat}}$ ; coupling g; lattice spacing a; electric field  $l_0 = rac{ heta}{2\pi}$ 

> mass shift MS :

 $m_r/g = m_{\text{lat}}/g + \text{MS}\left(V, ag, l_0\right)$ 

 $\rightarrow$  needs to be determined non-perturbatively

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# Pauli representation through Jordan-Wigner transformation

> Jordan-Wigner transformation

$$\begin{split} \phi_{n,\alpha} &\to \chi_{2n-\lfloor\frac{\alpha}{2}\rfloor+1} \\ \chi_n &= \prod_{k < n} (iZ_k) \sigma_n^- \end{split}$$

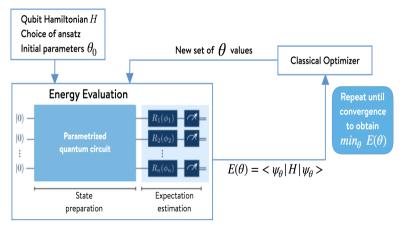
> (dimensionless) Wilson Hamiltonian,  $x = 1/(ag)^2$  $\rightarrow$  open boundary conditions: eliminate gauge fields

$$W_W = x \sum_{n=0}^{N-2} \left( X_{2n+2} X_{2n+3} + Y_{2n+2} Y_{2n+3} \right) + \left( \frac{m_{\text{lat}}}{g} \sqrt{x} + x \right) \sum_{n=0}^{N-1} \left( X_{2n+1} X_{2n+2} + Y_{2n+1} Y_{2n+2} \right) + \sum_{n=0}^{N-2} \left( l_0 + \sum_{k=0}^n Q_k \right)^2$$

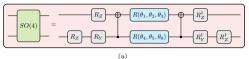
see also talk by M. Honda based on Digital Quantum Simulation for Spectroscopy of Schwinger Model, D. Ghim and M. Honda, arxiv:2404.14788

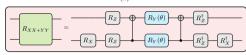
### Variational Quantum Eigensolver (VQE)

> a hybrid quantum/classical variational approach

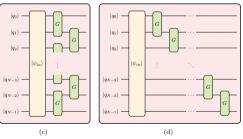


### **The Ansatz**









• decomposition of SO(4) and  $R_{XX+YY}$  gates

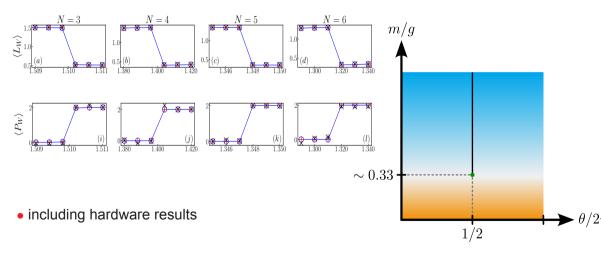
• brick and ladder ansatz

### **Results: small mass**

> results for  $m_r/q = 0.01$  (remember:  $x = 1/(aq)^2$ ) m/a0.0100 0.0075 0.0050 Mass perturbation theory 0.0025F Staggered with theory MS (same num. of qubits as Wilson). MSE = 5.989e-07Staggered (same x as Wilson), MSE = 9.804e-09q0.0000 Staggered with theory MS (same x as Wilson), MSE = 9.816e-07Staggered (same num, of qubits as Wilson), MSE = 2.787e-08 Wilson, MSE = 3.581e-09-0.0025 + \* $\sim 0.33$ -0.0050-0.0075-0.0100 $\theta/2$ 0.2 0.3 0.4 0.5 0.6 0.7 0.1 1/2Lo

• blue circles: exact diagonalization, red pluses: exact simulations, black crosses: IBM quantum hardware

### **Results: large mass** $m_r/g = 10$

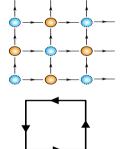


### The Hamiltonian of 2+1 dimensional QED

> fermionic matter fields on lattice sites

$$\hat{H}_{kin} = \frac{i}{2} \sum_{\vec{n}} \left( \phi_{\vec{n}}^{\dagger} \hat{U}_{\vec{n},x} \phi_{\vec{n}+x} - h.c. \right) - \frac{(-1)^{n_x + n_y}}{2} \sum_{\vec{n}} \left( \phi_{\vec{n}}^{\dagger} \hat{U}_{\vec{n},y} \phi_{\vec{n}+y} + \text{ h.c. } \right)$$

- $\hat{H}_m = m \sum_{\vec{n}} (-1)^{n_x + n_y} \hat{\phi}_{\vec{n}}^{\dagger} \hat{\phi}_{\vec{n}}$
- > set "bare" lattice spacing a = 1, physical a = a(g)
- > electric field and plaquette operators  $\hat{H}_E = \frac{g^2}{2} \sum_{\vec{n}} \left( \hat{E}_{\vec{n},x}^2 + \hat{E}_{\vec{n},y}^2 \right), \quad \hat{H}_B = -\frac{1}{2g^2} \sum_{\vec{n}} \left( \hat{P}_{\vec{n}} + \hat{P}_{\vec{n}}^\dagger \right)$
- > plaquette operator  $\rightarrow$  magnetic effects  $\hat{P}_{\vec{n}} = \hat{U}_{\vec{n},x} \hat{U}_{\vec{n}+x,y} \hat{U}_{\vec{n}+y,x}^{\dagger} \hat{U}_{\vec{n},y}^{\dagger}$



# Static potential from a quantum computer

static potential in 2+1-dimensional QED

 $V(r) = c_1 + c_2 \alpha(r) \ln(r) + c_3 \sigma r$ 

- $\alpha(r)$  running coupling
- $-\sigma$  string tension
- fixed distance in lattice units
- lattice spacing a ↘ when g ↘
   → physical distance
   becomes smaller

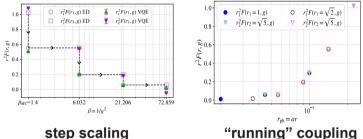
 > flux configurations at different disctances
 → see talk by Enrico Rinaldi

# Running coupling from MC and QC

(A. Crippa, S. Romiti, L. Funcke, K. Jansen, S. Kühn, P. Stornati, C. Urbach, arXiv:2404.17545)

 $\rightarrow$  see poster

QC: step scaling at very small lattice spacing
 MC: provide value of lattice spacing



Simulating 2D lattice gauge theories on a qudit quantum computer (M. Meth, J. Haase, J. Zhang, C. Edmunds, L. Postler, A. Steiner, A. Jena, L. Dellantonio, R. Blatt, P. Zoller, T. Monz, P. Schindler, C. Muschik, M. Ringbauer, arXiv:2310.12110) (Quantum Computing: a future perspective for scientific computing | Karl Jansen | Calims, The XVIth Quark Confinement and the Hadron Spectrum Conference, 19.8.2024 Page 2

# Chern-Simons term in 2+1 dimensional QED

(C. Peng, C. Diamantini, L. Funcke, A. Hassan, K. Jansen, Stefan Kühn, D. Luo, P. Naredi, arxiv:2407.20225)

$$\hat{H} = \sum_{x \in \text{ sites }} \frac{e^2}{2a^2} \left[ \left( \hat{p}_{x;1} - \frac{ka^2}{4\pi} \hat{A}_{x-\hat{2};2} \right)^2 + \left( \hat{p}_{x;2} + \frac{ka^2}{4\pi} \hat{A}_{x-\hat{1};1} \right)^2 \right] + \frac{1}{2e^2} \left( \Box \hat{A}_{x;1,2} \right)^2$$
energy bands
$$\int_{-2}^{-2} \int_{0}^{2} \int_{0}^$$

### pure Maxwell theory massless photon

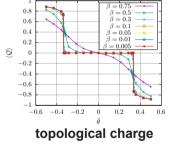
adding Chern-Simons term topological mass generation

> opens door to investigate e.g. fermion/boson dualities, fractional quantum Hall effect,

### Topological term in 3+1 dimensional compact QED

(A. Kan, L. Funcke, S. Kühn, L. Dellantonio, J. Zhang, J Haase, C. Muschik, K. Jansen, arxiv:2105.06019)

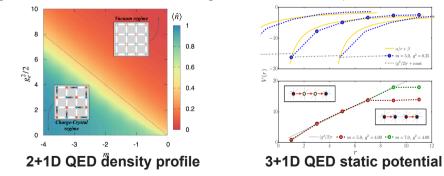
$$\hat{H}_{\text{topo}} = \tilde{\theta} \hat{Q} = -i\frac{\theta}{\beta} \sum_{\vec{n}} \sum_{(i,j,k) \in \text{ even }} \left( \hat{E}_{\vec{n}-\hat{i},i} + \hat{E}_{\vec{n},i} \right) \left( \hat{U}_{\vec{n},jk} - \hat{U}_{\vec{n},jk}^{\dagger} \right)$$



- 1st order phase transition for  $\beta < 1$
- observe avoided level crossing

### Higher dimension tensor network QED simulations

- > 2+1 dimensional QED at finite density on up to 16 x 16 lattices (T. Felser, P. Silvi, M. Collura, S. Montangero, arxiv:1911.09693)
- 3+1 dimensional QED at finite charge density
   G. Magnifico, T. Felser, P. Silvi, S. Montangero, arxiv:2011.10658)



### **Overview**



### > Non-abelian gauge theories

### Non-abelian lattice gauge theory

$$\begin{split} \hat{H} &= \frac{1}{2a} \sum_{\vec{n}} \sum_{\alpha,\beta} \left( i \hat{\psi}_{\alpha}(\vec{n})^{\dagger} \hat{U}_{\alpha\beta}(\vec{n},i) \hat{\psi}_{\beta}(\vec{n}+\hat{i}) + (-1)^{\vec{n}} \hat{\psi}_{\alpha}(\vec{n})^{\dagger} \hat{U}_{\alpha\beta}(\vec{n},j) \hat{\psi}_{\beta}(\vec{n}+\hat{j}) + \text{ H.c. } \right) \\ &+ m \sum_{\vec{n}} \sum_{\alpha} (-1)^{\vec{n}} \hat{\psi}_{\alpha}^{\dagger}(\vec{n}) \hat{\psi}_{\alpha}(\vec{n}) \\ &+ \frac{g^2}{2a^{d-2}} \sum_{\vec{n},l} \sum_{b} \left[ \hat{E}^{b}(\vec{n},l) \right]^2 \\ &- \frac{1}{2a^{4-d}g^2} \sum_{\vec{n}} \sum_{\alpha,\beta,\gamma,\delta} \hat{U}_{\alpha\beta}(\vec{n},i) \hat{U}_{\beta\gamma}(\vec{n}+\hat{i},j) \hat{U}_{\delta\gamma}^{\dagger}(\vec{n}+\hat{j},i) \hat{U}_{\alpha\delta}^{\dagger}(\vec{n},j) + \text{ H.c. } \end{split}$$

• Isn't it a nice Hamiltonian?

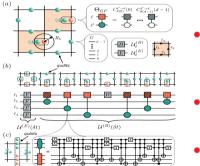
н.



# SU(2) LGT for qudit architecture

> quditing SU(2)

(D. González-Cuadra, T. Zache, J. Carrasco, B. Kraus, P. Zoller, arxiv:2203.15541)



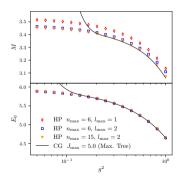
• Rydberg atoms for qudits

- qudit circuit
- comparing to qubit circuit
- promising realization of SU(2) q-deformed Kogut-Susskind gauge theories
  - (T. Zache, D. González-Cuadra, P. Zoller, arXiv:2304.02527)

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### Non-abelian lattice gauge theory

- > approach of SU(2) partitionings
- Hermite polynomial based operators
   (M. Garofalo, T. Hartung, T. Jakobs, K. Jansen, J. Ostmeyer, S. Romiti and C. Urbach, to appear)



- $E_0$  ground state
- M mass gap
- solid curve:

character expansion with electric operators

• data points:

hermite polynomial based operators

### Other approaches, non exhaustive examples ...

- > Non-abelian gauge theories in optical lattices
  - L.Tagliacozzo, A.Celi, P.Orland, M. Mitchell, M. Lewenstein, Nature communications, 4(1):1–8, 2013
- > Clebsch-Gordaning
  - N. Klco, M. Savage, and J. Stryker, Physical Review D, 101(7):074512
  - Sarmed Rahman, Randy Lewis, Emanuele Mendicelli, Sarah Powell, Phys. Rev. D 104, 034501 (2021)
- > Integrating out gauge fields
  - Y. Atas, J. Haase, J. Zhang, V. Wei, S. Pfaendler, R. Lewis, and C. Muschik, arXiv:2207.03473
  - Y. Atas, J. Haase, J. Zhang, V. Wei, S. Pfaendler, R. Lewis, and C. Muschik, Nature communications, 12(1):1–11, 2021
- > General quantum algorithm approach
  - Z. Davoudi, A. Shaw, J. R. Stryker, arXiv:2212.14030v2
- Highly-efficient quantum Fourier transformations for some nonabelian groups E. Murairi, M. Alam, H. Lamm, S. Hadfield, E. Gustafson, arXiv:2408.00075

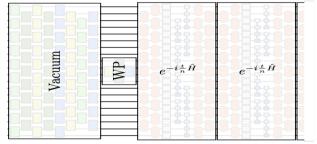
### **Overview**



### > Real time dynamics

#### real time dynamics

- > Common scheme for real time dynamics
  - ground state preparation of considered model
  - generate hadron wavepacket on the ground state
  - real time evolution of the wave packet
  - measurement of relevant observables
- algorithms:
   VQE, Trotterization,
   Givens rotation, ...
- ansätze: brick, ladder, charge conservation, ...



# **Quantum Simulations of Hadron Dynamics in the Schwinger Model**

(R. Farrell, M. Illa, A. Ciavarella, M. Savage, arXiv:2401.08044)

#### ground state preparation:

- use locality of interaction: effective Hamiltonian
- Scalable Circuits-ADAPT-VQE (SC-ADAPT-VQE) algorithm: → define pool of operators  $\{\hat{O}\}_{\text{vac}} = \left\{\hat{O}_{mh}^{V}(d), \hat{O}_{mh}^{S}(0, d), \hat{O}_{mh}^{S}(1, d)\right\}$

$$\hat{O}_{mh}^{V}(d) \equiv i \left[ \hat{\Theta}_{m}^{V}, \hat{\Theta}_{h}^{V}(d) \right] = \frac{1}{2} \sum_{n=0}^{2L-1-d} (-1)^{n} \left( \hat{X}_{n} \hat{Z}^{d-1} \hat{Y}_{n+d} - \hat{Y}_{n} \hat{Z}^{d-1} \hat{X}_{n+d} \right)$$

$$\hat{\mathcal{Q}}_{mh}^{S}(0,d) \equiv i \left[ \hat{\Theta}_{m}^{S}(0), \hat{\Theta}_{h}^{V}(d) \right] = \frac{1}{4} \left( \hat{X}_{0} \hat{Z}^{d-1} \hat{Y}_{d} - \hat{Y}_{0} \hat{Z}^{d-1} \hat{X}_{d} - \hat{Y}_{2L-1-d} \hat{Z}^{d-1} \hat{X}_{2L-1} + \hat{X}_{2L-1-d} \hat{Z}^{d-1} \hat{Y}_{2L-1} \right)$$

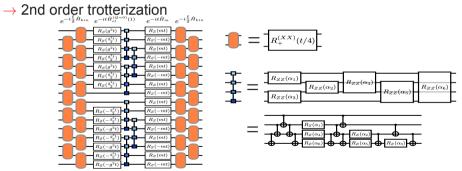
$$\hat{O}_{mh}^{S}(1,d) \equiv i \left[ \hat{\Theta}_{m}^{S}(1), \hat{\Theta}_{h}^{S}(d) \right] = \frac{1}{4} \left( \hat{Y}_{1} \hat{Z}^{d-1} \hat{X}_{d+1} - \hat{X}_{1} \hat{Z}^{d-1} \hat{Y}_{d+1} + \hat{Y}_{2L-2-d} \hat{Z}^{d-1} \hat{X}_{2L-2} - \hat{X}_{2L-2-d} \hat{Z}^{d-1} \hat{Y}_{2L-2} \right)$$

- rank the operators, e.g. according to infidelity
- perform all this on small lattices and extrapolate to large lattice
   demonstrated on 100 qubits in
   (D. Forroll, M. Illo, A. Cipurrolla, M. Source, arXiv:2208.04484)

(R. Farrell, M. Illa, A. Ciavarella, M. Savage, arXiv:2308.04481)

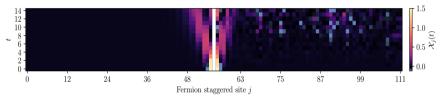
## **Quantum Simulations of Hadron Dynamics in the Schwinger Model**

- generate hadron wavepacket on the the ground state
  - $\rightarrow$  adiabatically evolving ground state
- real time evolution of the wave packet:

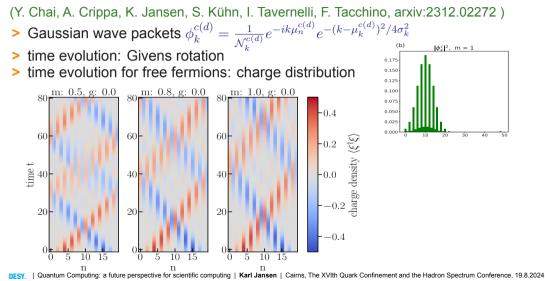


## **Quantum Simulations of Hadron Dynamics in the Schwinger Model on 112 qubits**

- measurement of relevant observables:
  - → chiral condensate

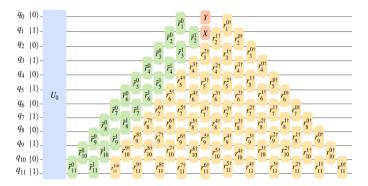


## Scattering in the Thirring model

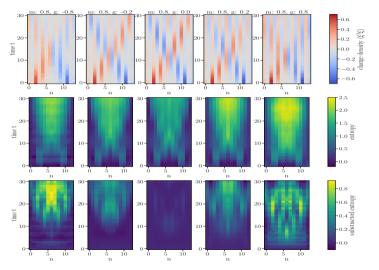


#### **Quantum circuit**

- > blue box: vacuum preparation
- > green and yellow boxes: wave packet preparation and time evolution

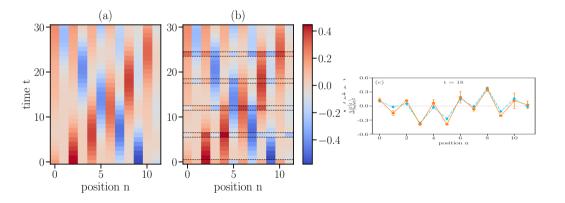


#### **Interacting case**



#### Hardware runs

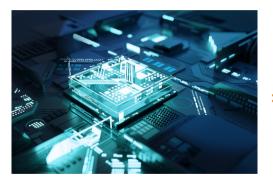
#### > Ideal versus hardware



#### Quantum computing real time evolution, not exhaustive

- > A Cold-Atom Particle Collider (Guo-Xian Su, Jesse Osborne, Jad C. Halimeh, arxiv:2401.05489)
- Meson Mass Sets Onset Time of Anomalous Dynamical Quantum Phase Transitions (Jesse J. Osborne, Johannes Knaute, Ian P. McCulloch, Jad C. Halimeh, arxiv:2407.03394)
- Quantum Computing Universal Thermalization Dynamics in a (2+1)D Lattice Gauge Theory (Niklas Mueller, Tianyi Wang, Or Katz, Zohreh Davoudi, Marko Cetina, arxiv:2408.00069)
- Simulating Meson Scattering on Spin Quantum Simulators (Elizabeth R. Bennewitz, Brayden Ware, Alexander Schuckert, Alessio Lerose, Federica M. Surace, Ron Belyansky, William Morong, De Luo, Arinjoy De, Kate S. Collins, Or Katz, Christopher Monroe, Zohreh Davoudi, Alexey V. Gorshkov, arXiv:2403.07061v2)
- > Applying the noiseless extrapolation error mitigation protocol to calculate real-time quantum field theory scattering phase shifts (Zachary Parks, Arnaud Carignan-Dugas, Erik Gustafson, Yannick Meurice, Patrick Dreher, arXiv:2212.05333)
- Real-time chiral dynamics at finite temperature from quantum simulation (Kazuki Ikeda, Zhong-Bo Kang, Dmitri E. Kharzeev, Wenyang Qian, Fanyi Zhao, arXiv:2407.21496)

#### **Overview**



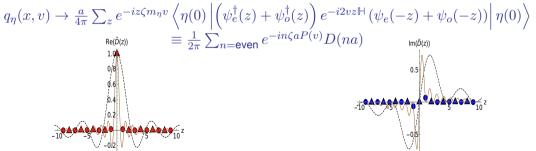
#### > PDFs

### Quantum computing parton distribution functions

- (S. Grieninger, K. Ikeda, I. Zahed), arXiv:2404.05112v1)
- > employing the Schwinger model Hamiltonian
- > parton distribution function from "time" evolution

 $q_{\eta}(x,v) = \frac{1}{2} \int_{-\infty}^{+\infty} \frac{dz}{2\pi} e^{-iz\zeta m_{\eta}v} \left\langle \eta(0) \left| \bar{\psi}(0,z)[z,-z] \gamma^{+} \gamma^{5} e^{-i2vz\mathbb{H}} \psi(0,-z) \right| \eta(0) \right\rangle$ 

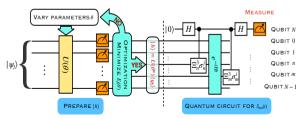
> staggered form on the lattice ( $\zeta = 2x - 1$ )



### Quantum computing parton distribution functions

- related work
  - Parton Physics on a Quantum Computer,
    - (H. Lamm, S. Lawrence, Y. Yamauchi, arXiv:1908.10439)
  - Quantum Simulation of Light-Front Parton Correlators, (M.G. Echevarria, I.L. Egusquiza, E. Rico, G. Schnell, arXiv:2011.01275v2)
  - Partonic collinear structure by quantum computing, (T. Li, X. Guo, W. Kin Lai, X. Liu, E. Wang, H. Xing, D. Zhang, S. Zhu, arXiv:2106.03865)
  - work on distribution amplitudes,

(T. Li, X. Guo, W. Kin Lai, X. Liu, E. Wang, H. Xing, D. Zhang, S. Zhu, arXiv:2207.13258 )



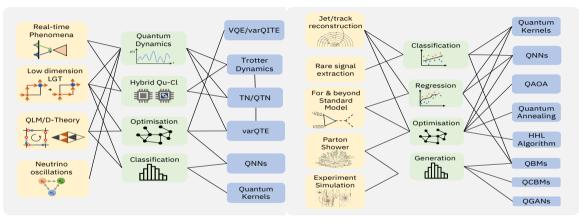
#### QC4HEP whitepaper, arXiv:2307.03236

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#### Abstract

Quantum computers offer an intriguing path for a paradigmatic change of computing in the natural sciences and beyond, with the potential for achieving a so-called quantum advantage, namely a significant (in some cases exponential) speed-up of numerical simulations. In particular, the high-energy physics community plays a pivotal role in accessing the power of quantum computing, since the field is a driving source for challenging computational problems. ...

### Algorithms, methods and application for HEP



## TheoryExperimentSee also Quantum Simulation for High-Energy Physics, C. Bauer et.al., arxiv:2204.03381

## QC for high energy, nuclear and condensed matter physics

Leaving the era of 1+1 dimensional toy models



- abelian and non-abelian pure gauge theories in 2 space dimensions
- > QED in 2+1 dimensions
- > abelian Higgs model
- > topological terms → CP-violation
- > PDFs for simple models



- abelian and non-abelian gauge theories in 3 space dimensions
- > QED in 3+1 dimensions
- > non-abelian Higgs model
- topological terms
   topological materials



- SU(2) and SU(3) 'QCD' in 2+1 and 3+1 dimensions
- > QCD with topological term
- > chiral gauge theories
- extensions of standard model
- > non-zero matter density

## QC for high energy, nuclear and condensed matter physics

Leaving the era of 1+1 dimensional toy models



- real time simulation → thermalization
  - $\rightarrow$  scattering
  - $\rightarrow$  quenching

>

- > various spin models
- > thermal field theory



- > real time simulation → string breaking, formation of bound states
- > collisions, scattering
- > non-perturbative renormalization

> ...



- simulations of heavy ion collisions
- > quark gluon plasma
- > nuclear physics

>

- > multi-Higgs models
- > conformal field theories

#### $\Rightarrow$ Completely new insight in condensed matter and high energy physics!

#### Thank you!





#### Contact

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