Scattering wave packets of hadrons in gauge theories: Preparation on a quantum computer

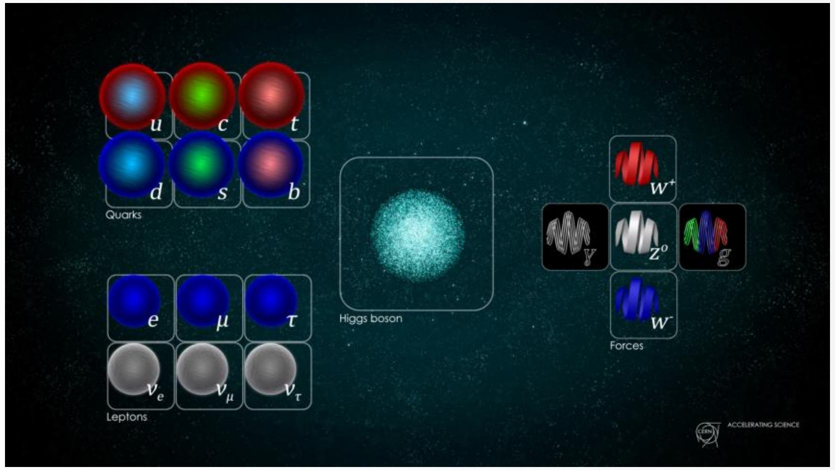
Chung-Chun Hsieh

with Prof. Zohreh Davoudi, Saurabh Kadam

Based on arXiv:2402.00840 [quant-ph]

Introduction

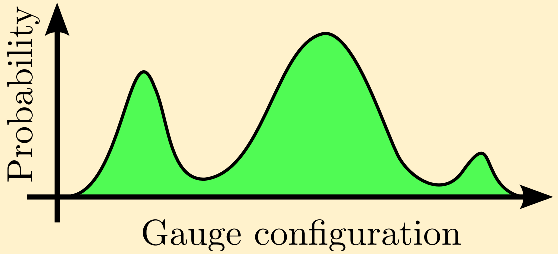
Photo credit: CERN



- Gauge theory
  - Standard model: $SU(3)_C \times SU(2)_L \times U(1)_Y$
  - Strongly interacting (e.g. QCD at low energy): non-perturbative methods
  - Real-time processes hard for lattice QCD

- Lattice QCD

$$\langle \hat{\boldsymbol{O}} \rangle = \frac{1}{Z} \int \mathcal{D}[\bar{\psi}, \psi] \mathcal{D}[A] \hat{\boldsymbol{O}} e^{-\int d^4 x_E \mathcal{L}_E}$$



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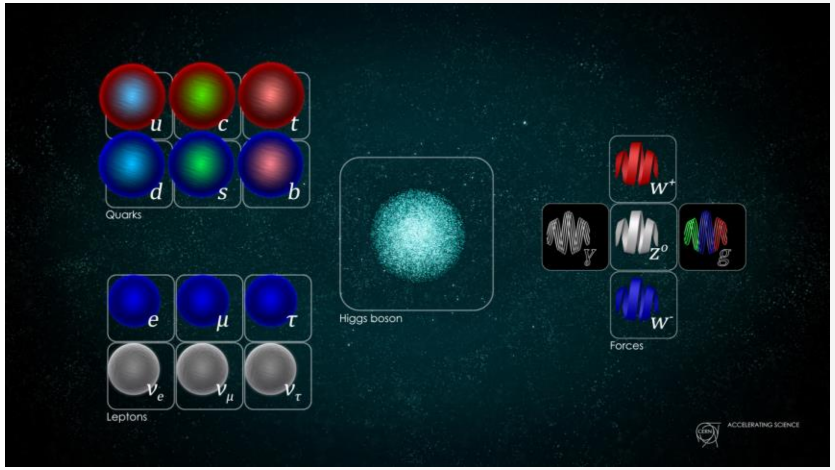

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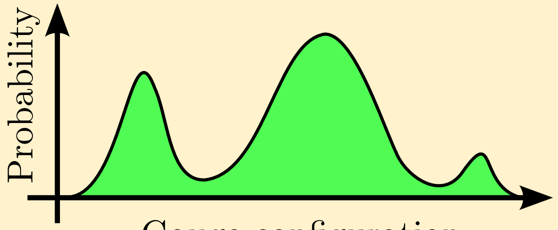


- Hamiltonian formulation

$$\langle \hat{\boldsymbol{O}}(\boldsymbol{t}) \rangle = \langle 0 | e^{iHt} \hat{\boldsymbol{O}}(\boldsymbol{0}) e^{-iHt} | 0 \rangle$$

  - Exponential growth of Hilbert space

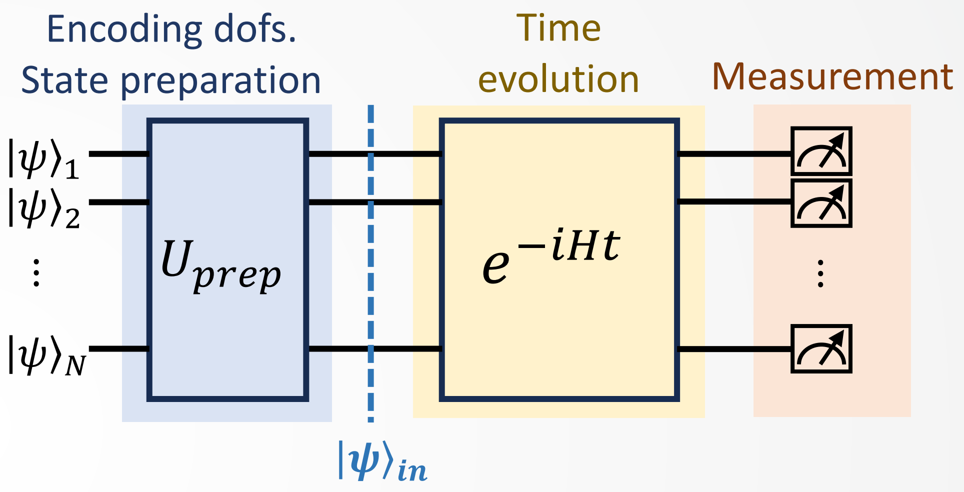
- Quantum simulation

$$|\psi\rangle = \cos(\theta/2)\,|0\rangle + e^{-i\phi} \sin(\theta/2)\,|1\rangle$$

$$|\psi\rangle_1 \otimes |\psi\rangle_2 \otimes \cdots \otimes |\psi\rangle_N \sim 2^N$$

Quantum simulation

- Quantum simulation protocol:



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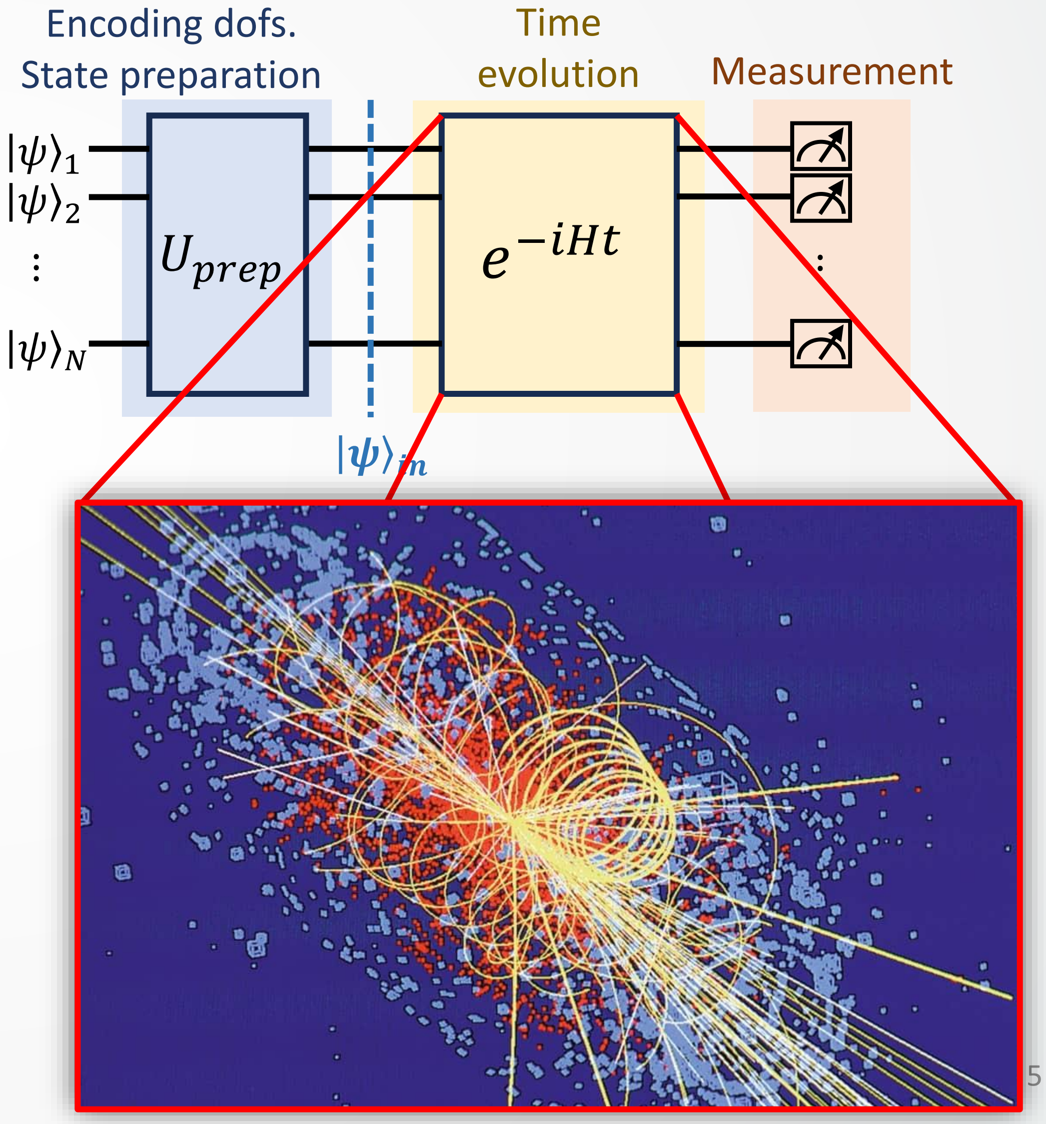

Photo credit: ATLAS

Quantum simulation

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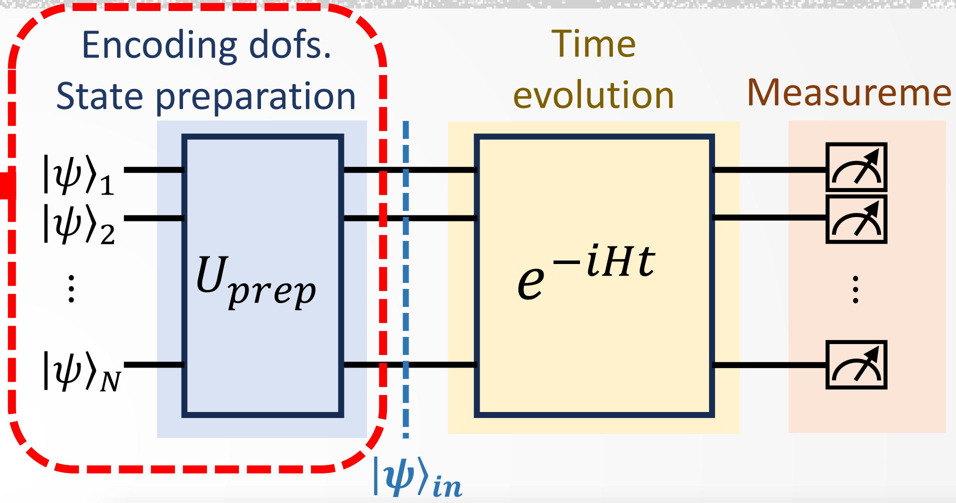


- Initial state for scattering: **interacting wave packets**, e.g.

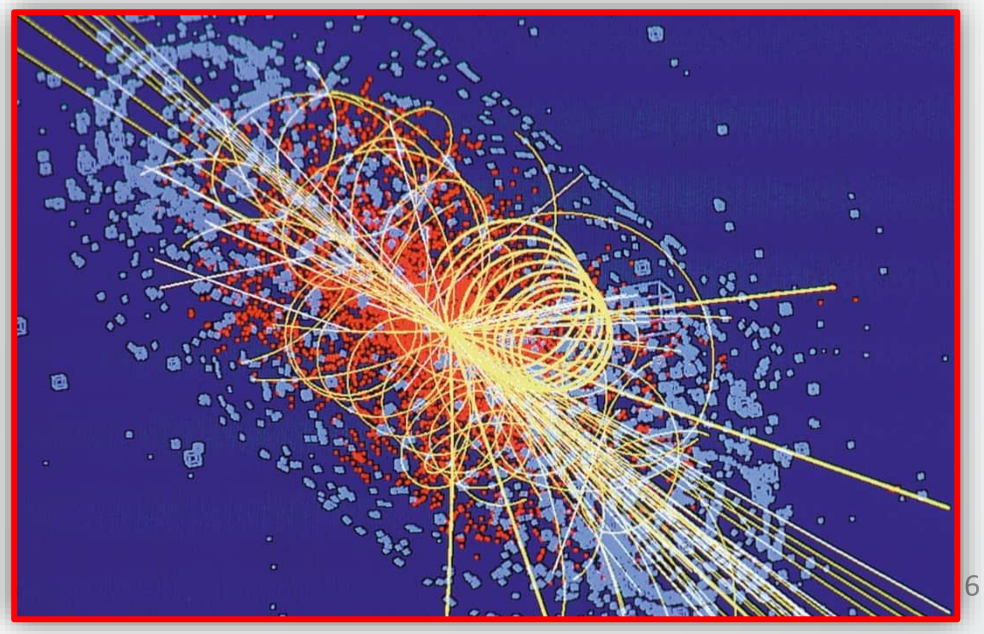
$$|\Psi\rangle = \sum_{k} \Psi(k)|k\rangle$$

Interacting momentum eigenstate

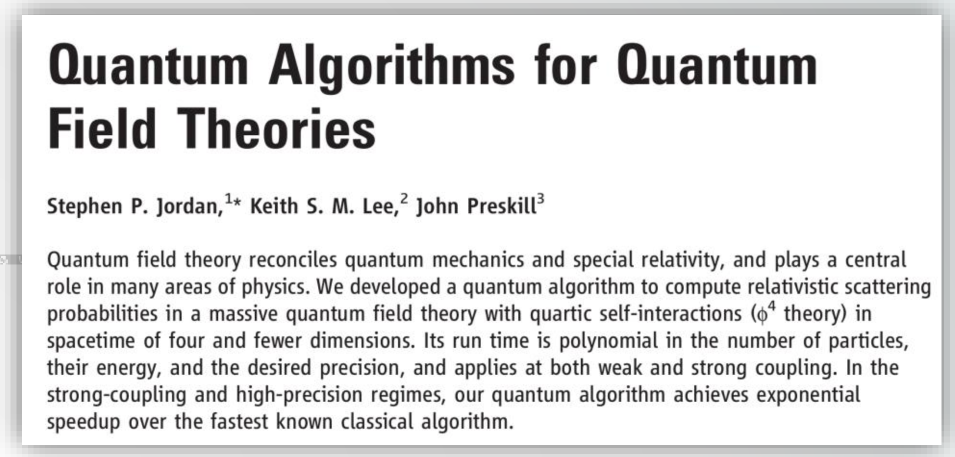
Wave-packet function

- State preparation can be challenging in quantum computing!

J. Kempe, A. Kitaev, O. Regev, FSTTCS 2004



JLP and alternatives

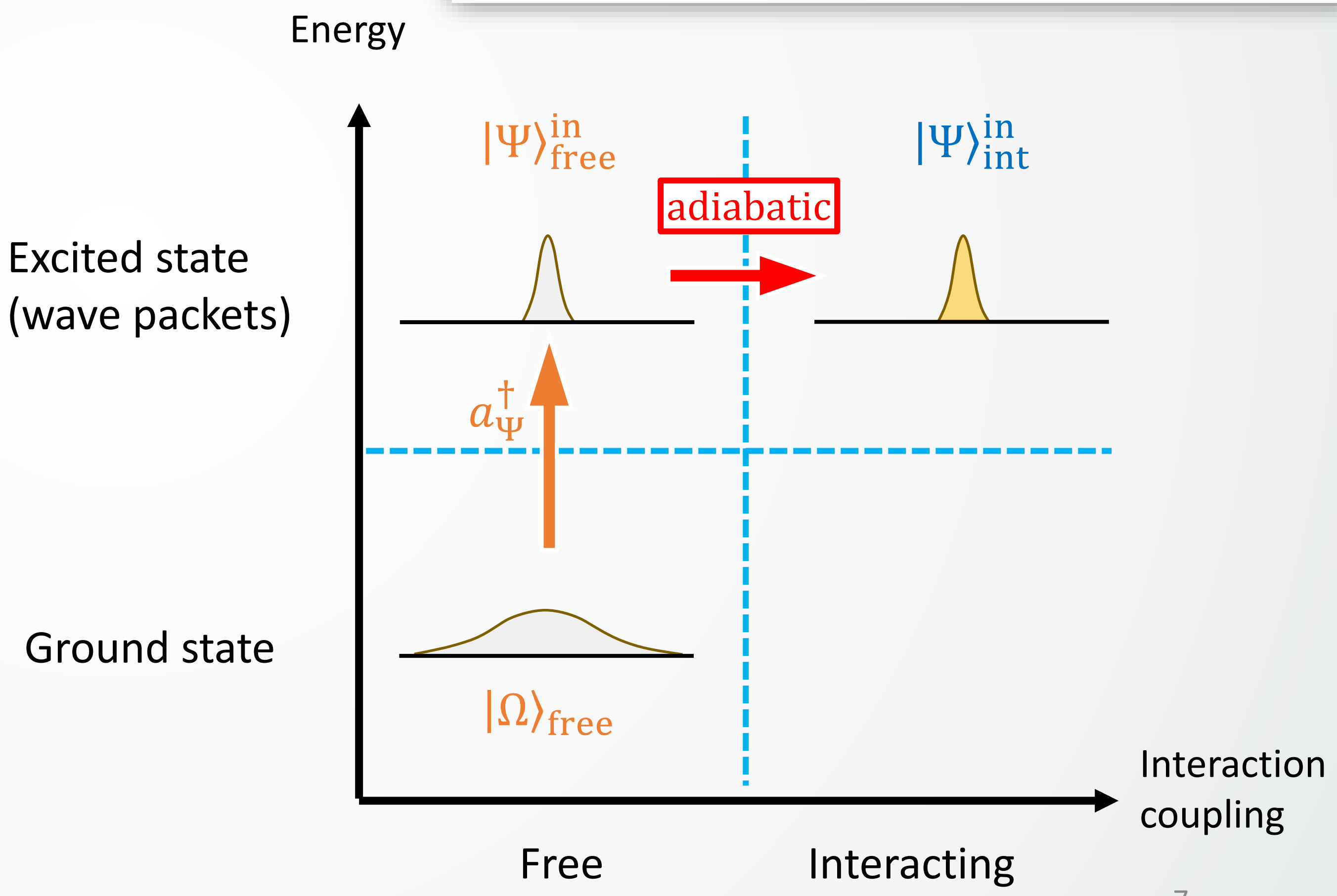

Quantum Algorithms for Quantum Field Theories

Stephen P. Jordan,[1*] Keith S. M. Lee,[2] John Preskill[3]

Quantum field theory reconciles quantum mechanics and special relativity, and plays a central role in many areas of physics. We developed a quantum algorithm to compute relativistic scattering probabilities in a massive quantum field theory with quartic self-interactions (ϕ^4 theory) in spacetime of four and fewer dimensions. Its run time is polynomial in the number of particles, their energy, and the desired precision, and applies at both weak and strong coupling. In the strong-coupling and high-precision regimes, our quantum algorithm achieves exponential speedup over the fastest known classical algorithm.

S. P. Jordan, K. S. M. Lee, and J. Preskill, Quantum algorithms for quantum field theories, Science 336, 1130 (2012)

- Jordan-Lee-Preskill:
  - **Adiabatic** activation of interaction
  - Resource intensive
  - Ineffective with phase transition, confinement



Digital

Adiabatic
- S. P. Jordan, K. S. M. Lee, J. Preskill, arXiv:1404.7115 [hep-th]
- J. Barata, N. Mueller, A. Tarasov, and R. Venugopalan, PRA 103, 042410
- T.D. Cohen and H. Oh, arXiv:2310.19229 [hep-lat]

Phase shift
- E. Gustafson, Y. Zhu, P. Dreher, N. M. Linke, and Y. Meurice, Phys. Rev. D 104, 054507 (2021)
- S. Sharma, T. Papenbrock, and L. Platter, arXiv:2311.09298 [nucl-th]

LSZ reduction
- T. Li, W. K. Lai, E. Wang, and H. Xing, Phys. Rev. D 109, 036025 (2024)
- R. A. Briceno, R. G. Edwards, M. Eaton, C. Gonzalez-Arciniegas, O. Pfister, and G. Siopsis, arXiv:2312.12613 [quant-ph]

Optical theorem
- A. Ciavarella, Phys. Rev. D 102, 094505 (2020)

Axiomatic QFT
- M. Turco, G. M. Quinta, J. Seixas, Y. Omar, PRX Quantum 5, 020311
- M. Kreshchuk, J. P. Vary, P. J. Love,arXiv:2310.13742 [quant-ph]

Fermionic excitation
- Y. Chai, A. Crippa, K. Jansen, S. Kuhn, V. R. Pascuzzi, F. Tacchino, and I. Tavernelli, arXiv:2312.02272 [quant-ph]

Adapt-VQE
- R. C. Farrell, M. Illa, A. N. Ciavarella, M. J. Savage, Phys. Rev. D 109, 114510 (2024)

Analog

Adiabatic
- A. N. Ciavarella, S. Caspar, M. Illa, M. J. Savage, Quantum 7, 970 (2023)

Non-Adiabatic
- F. M. Surace and A. Lerose, 2021 New J. Phys. 23 062001
- R. Belyansky, S. Whitsitt, N. Mueller, A. Fahimniya, E. R. Bennewitz, Z. Davoudi, A.V. Gorshkov, Phys. Rev. Lett. 132, 091903 (2024)

JLP and alternatives

M. Rigobello, S. Notarnicola, G. Magnifico, and S. Montangero, Phys. Rev. D 104, 114501 (2021)

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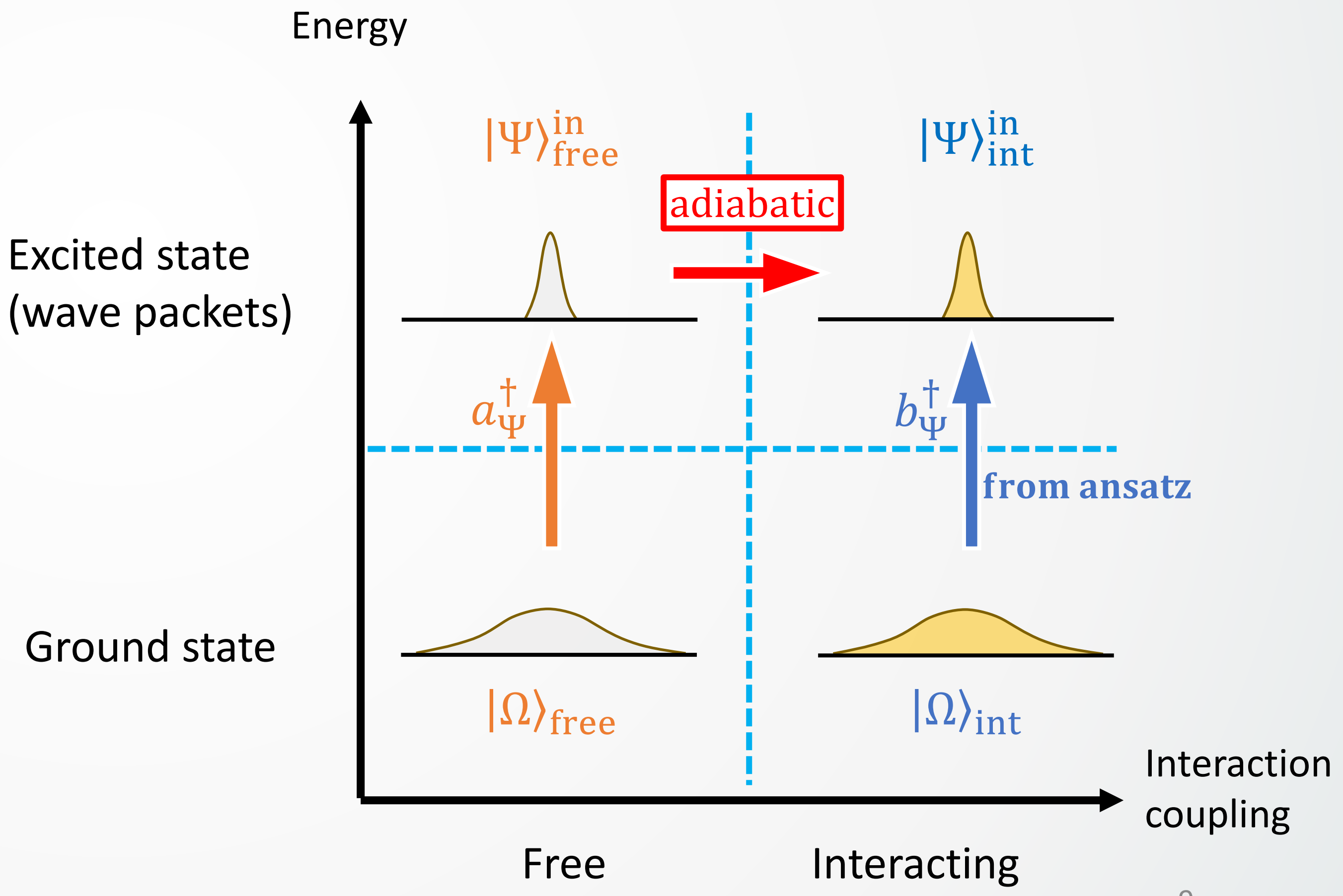
  - **Ansatz** based on the dofs of LGTs



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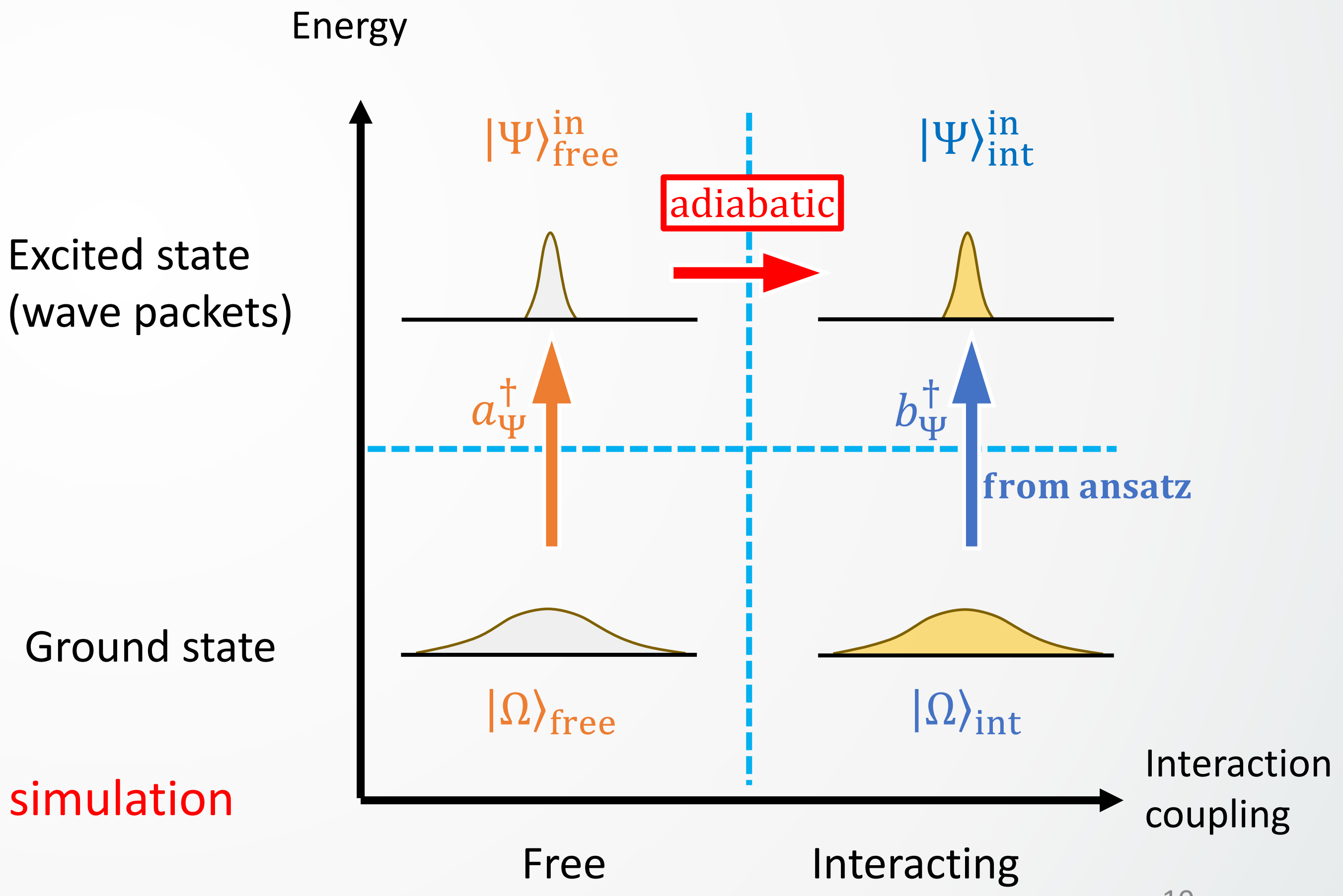


Bottom line:

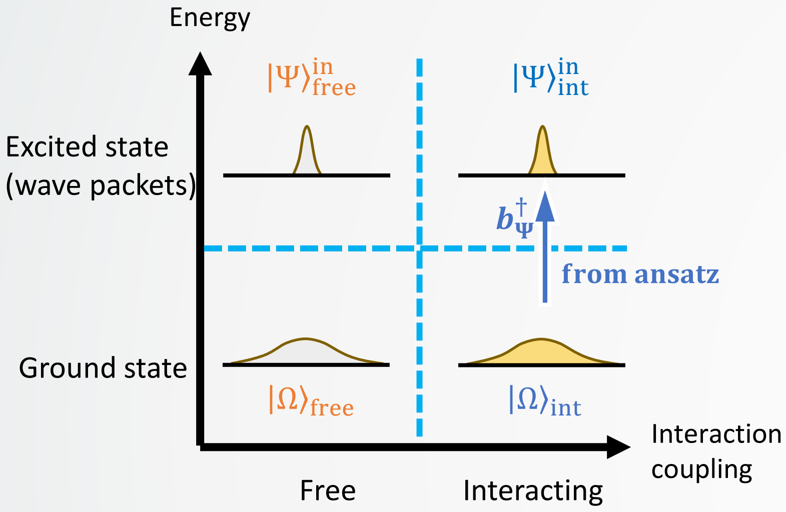
- Wave packet preparation is hard for quantum simulation
- We provide efficient algorithm & realization

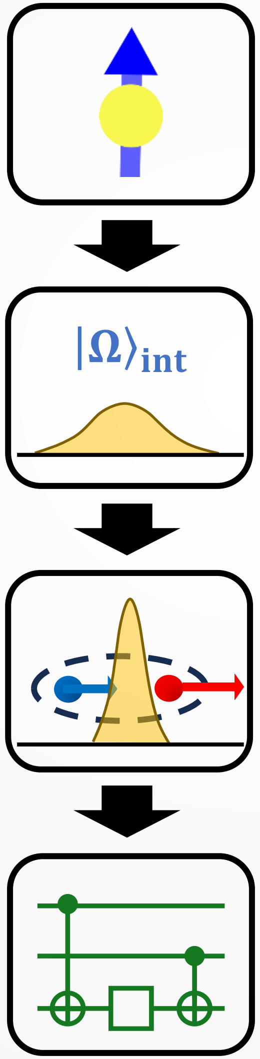
Outline

- Introduction
- **Quantum algorithm and circuit**
  - Model: 1+1D Z_2 LGT coupled to fermions
  - Ansatz for interacting wave-packet creation operator
  - Quantum circuit
- **Results**
  - Hardware: Quantinuum H1-1
- **Summary and Outlook**

Quantum algorithm and circuit

Algorithm





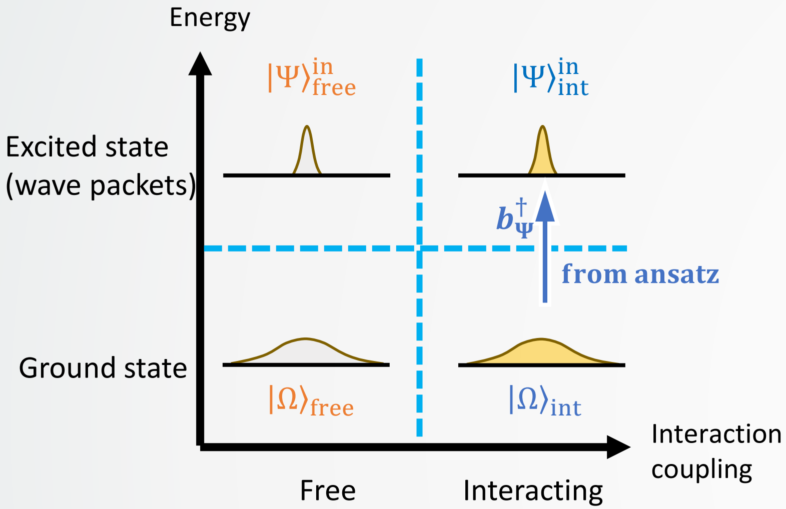
1. Mapping the degrees of freedom to qubits

2. Prepare the interacting ground state

3. Optimize an ansatz for creation operator

4. Quantum circuit for the wave packets

Algorithm

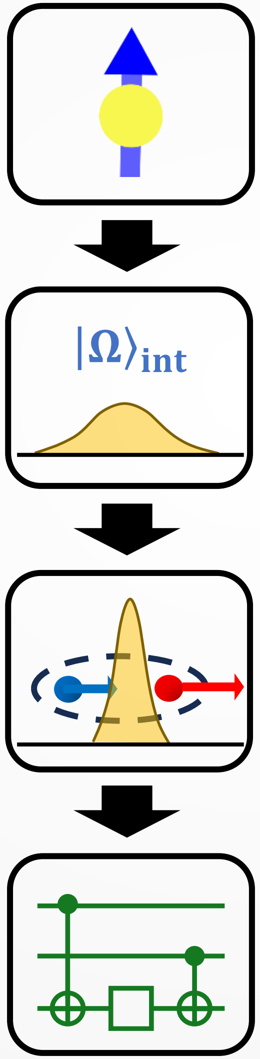


1+1D Z_2 LGT coupled to fermions (PBC)

$$H = \frac{1}{2}\sum_{n=0}^{N-1}\left(\xi_n^\dagger \xi_{n+a}\tilde{\sigma}_n^x + \text{H.c.}\right) + am_f\sum_{n=0}^{N-1}(-1)^{\frac{n}{a}}\xi_n^\dagger\xi_n + a\epsilon\sum_{n=0}^{N-1}\tilde{\sigma}_n^z$$

$$a = 1, N = 6$$

- The algorithm works with U(1) LGT. Only Z_2 is implemented on hardware due to resource limit



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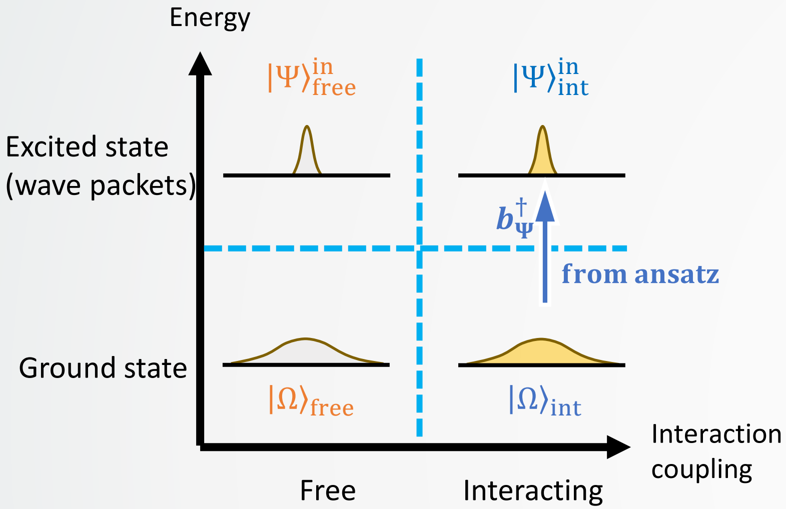
Algorithm: mapping to qubits



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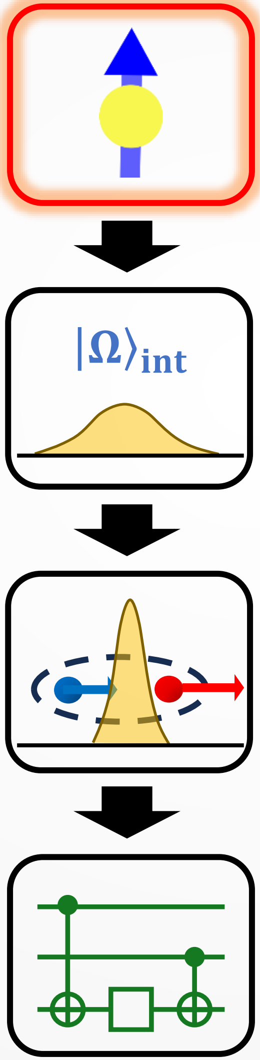
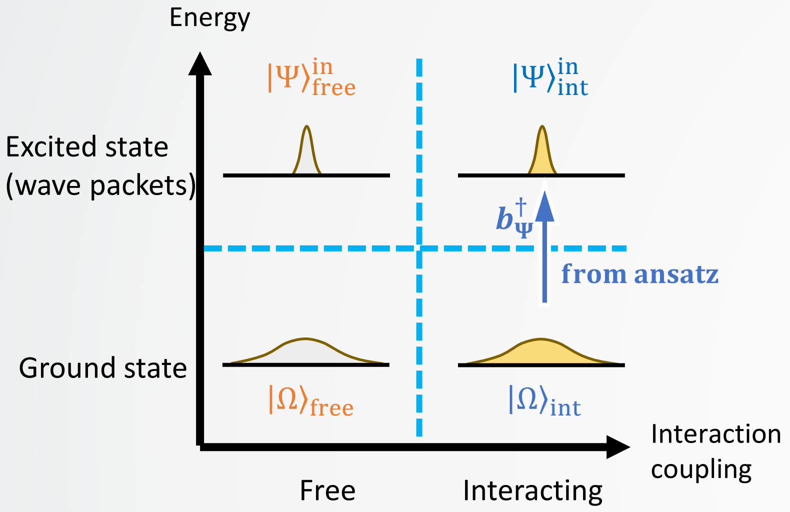
$$a = 1, N = 6$$

Mapping for fermions:

Jordan-Wigner: $\begin{cases} \xi_n^\dagger = \left(\prod_{j<n}\sigma_j^z\right)\sigma_n^- \\ \xi_n = \left(\prod_{j<n}\sigma_j^z\right)\sigma_n^+ \end{cases}$



Algorithm: Ground state preparation



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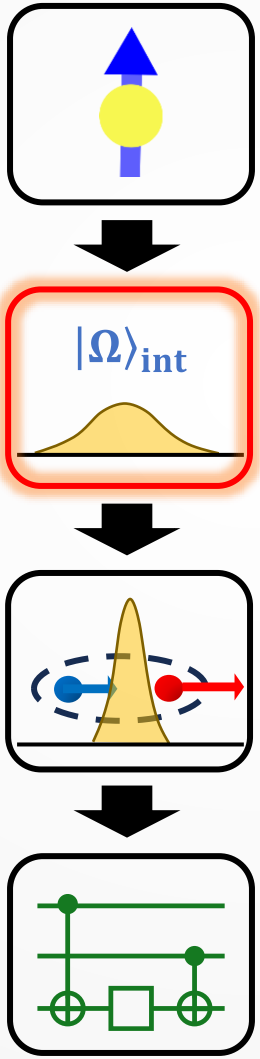
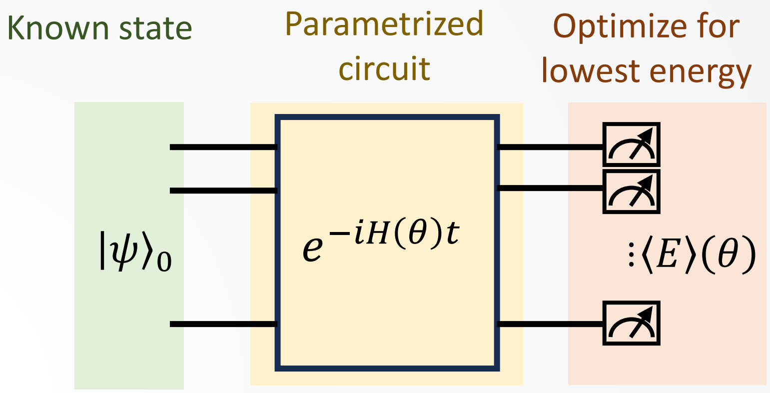
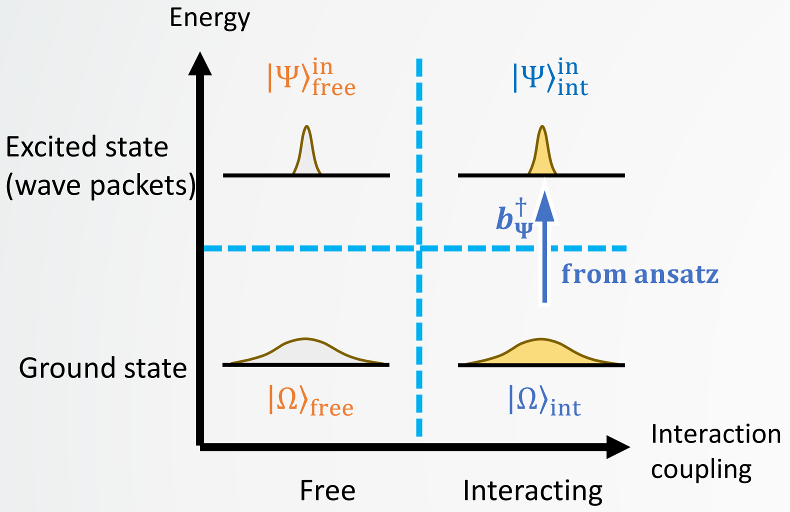




Variational Quantum Eigensolver (VQE)

Algorithm: Ground state preparation



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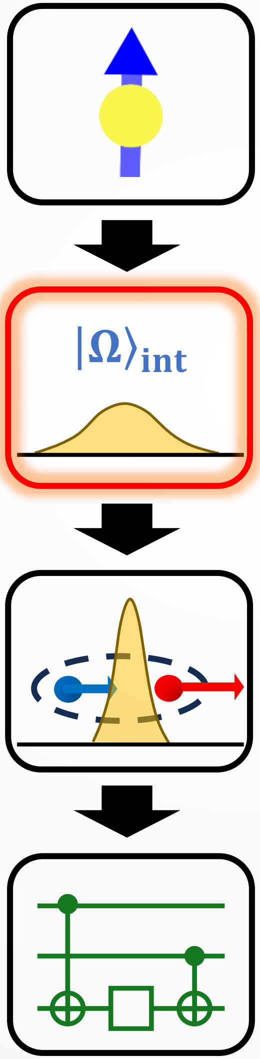
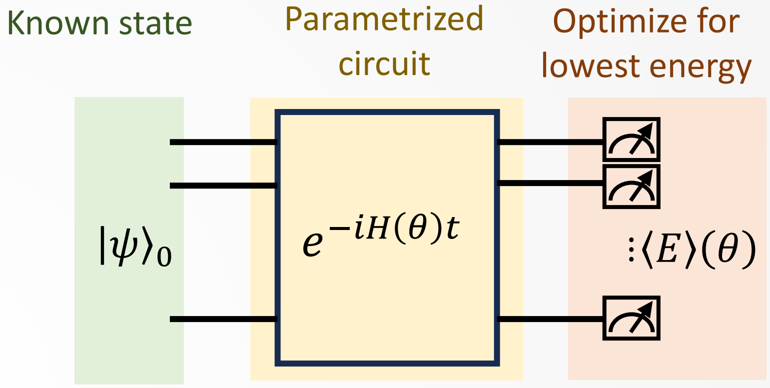
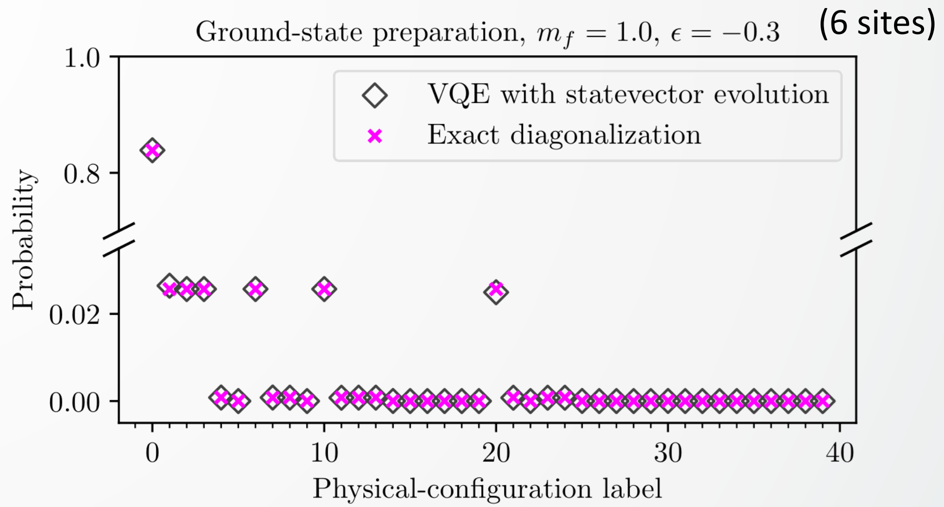


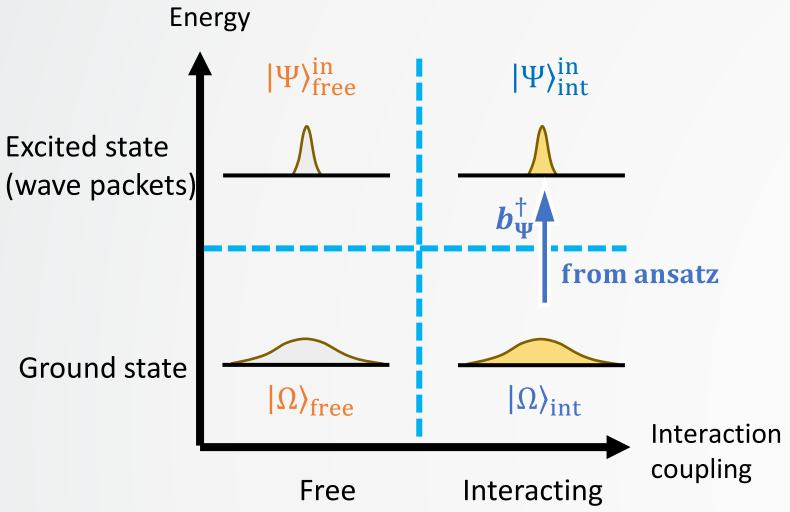


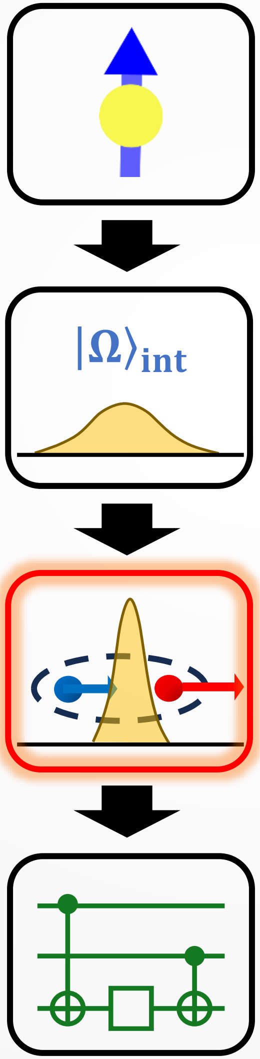
Variational Quantum Eigensolver (VQE)

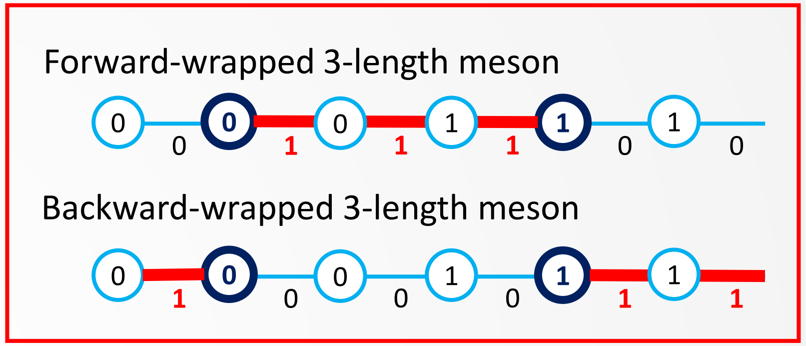


$$F_\Omega = \left|\langle \Omega_{exact} | \Omega_{optimized}\rangle\right|^2 \quad 1 - F_\Omega = 7.83 \times 10^{-5}$$

Algorithm: ansatz optimization







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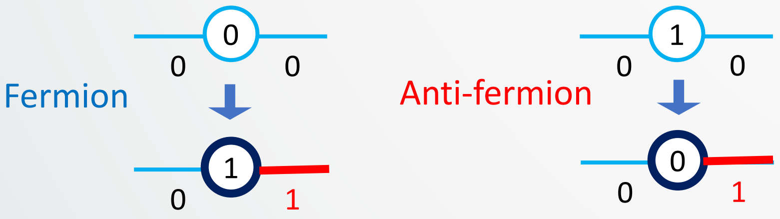
Gauss' law:



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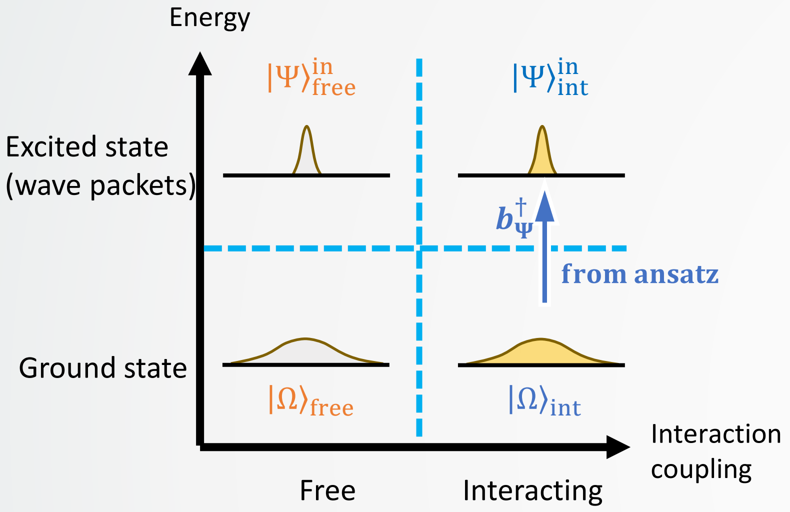
M. Rigobello, S. Notarnicola, G. Magnifico, and S. Montangero, Phys. Rev. D 104, 114501 (2021)



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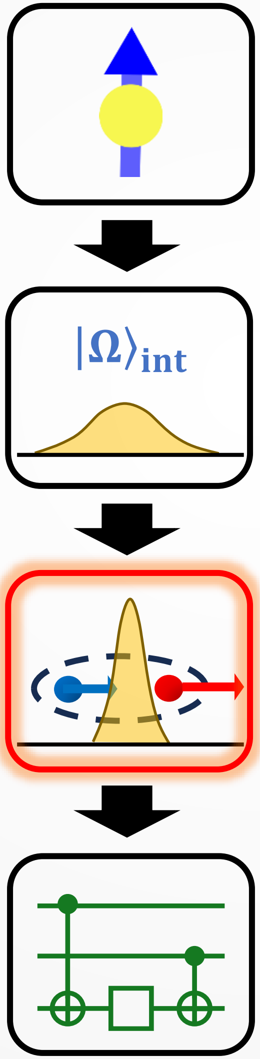

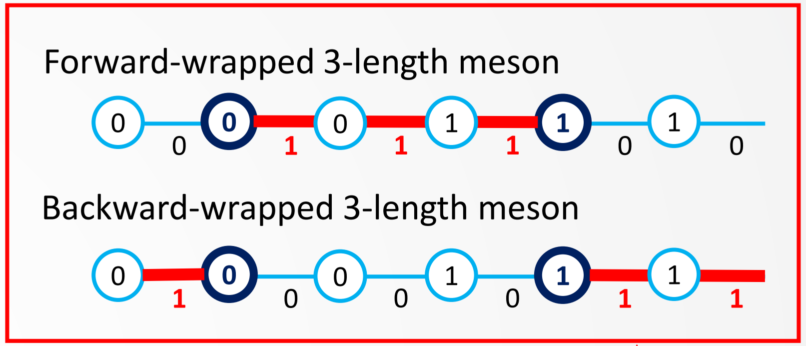

Fourier transform of $\xi^\dagger_m\left(\prod_{l=m}^{n-1}\tilde{\sigma}^x_l\right)\xi_n$

For each momentum k:

$$b^\dagger_k = \sum_{p,q\in\tilde{\Gamma}} \delta_{k-p-q}\,\eta(p,q)\,\mathcal{B}(p,q)$$

Conservation of momentum

Ansatz

Mesonic creation operator

$$\boldsymbol{b^\dagger_\Psi = \sum_k \Psi(k)\, b^\dagger_k}$$

Algorithm: ansatz optimization

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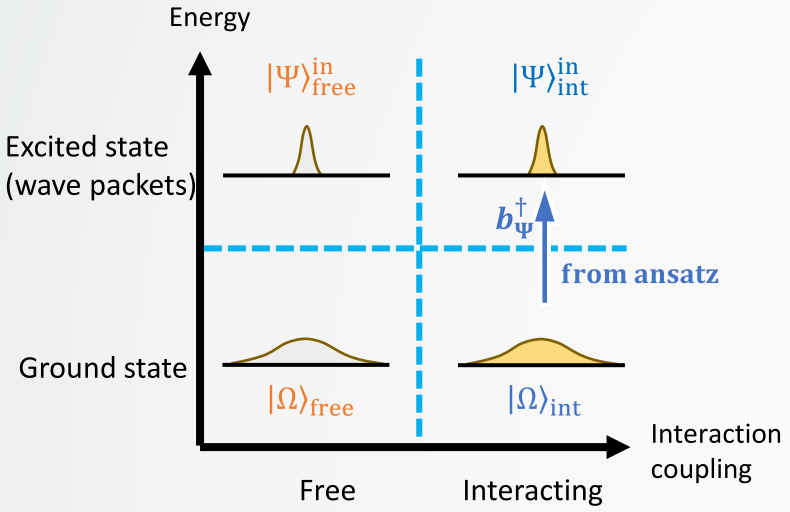

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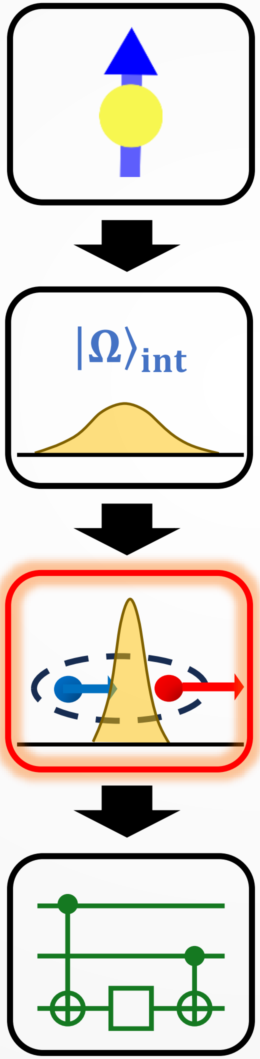

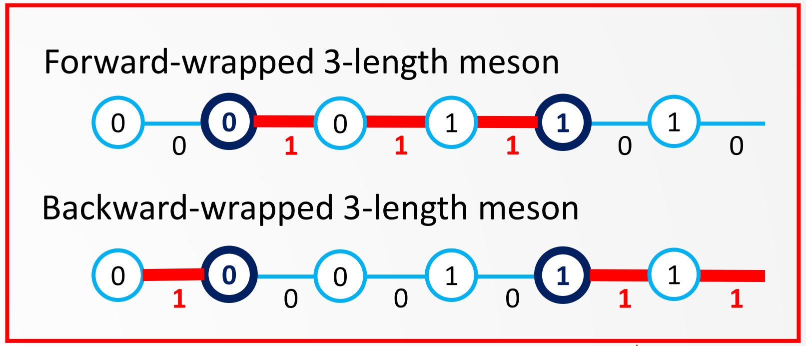

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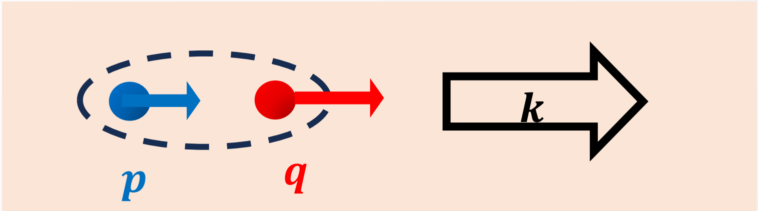
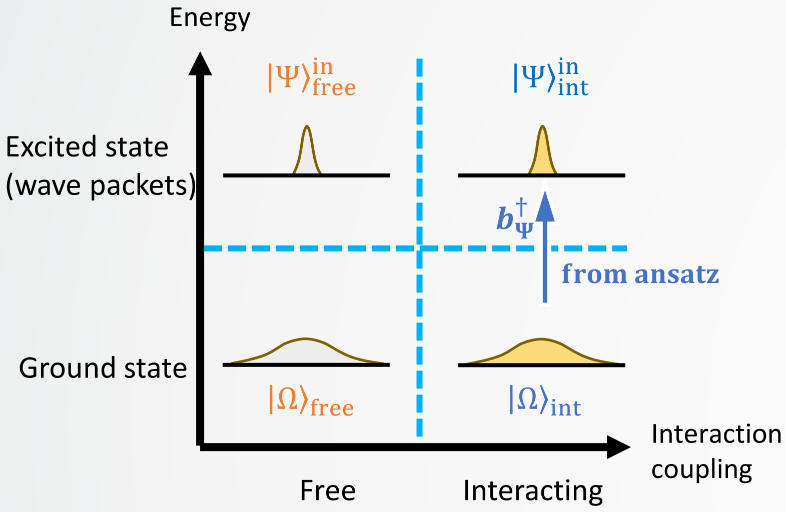


$$\eta(p,q) = N_\eta \exp\left(\frac{i(p-q)\mu^A_k}{2}\right)\exp\left(\frac{-(p-q)^2}{4{\sigma^A_k}^2}\right)$$

Optimize for lowest energy for each k

Algorithm: ansatz optimization



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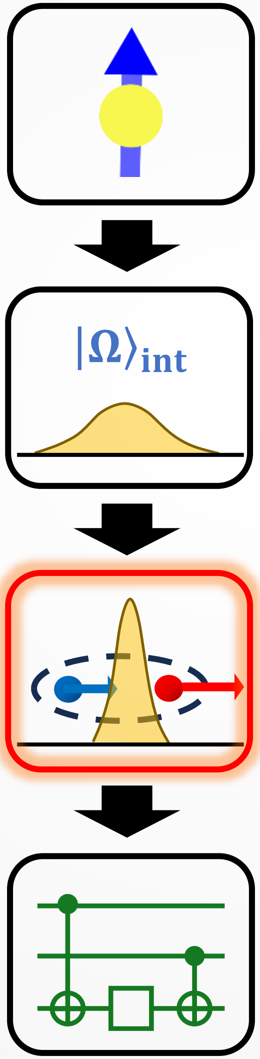
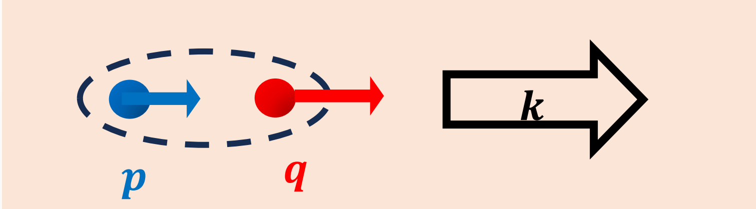


- **VQE** gives $|k\rangle$ (lowest energy other than ground state)
- Classical simulation of VQE in this work due to resource limit

For each momentum k:

$$b_k^{\dagger} = \sum_{p,q\in\tilde{\Gamma}} \delta_{k-p-q}\,\eta(p,q)\,\mathcal{B}(p,q)$$



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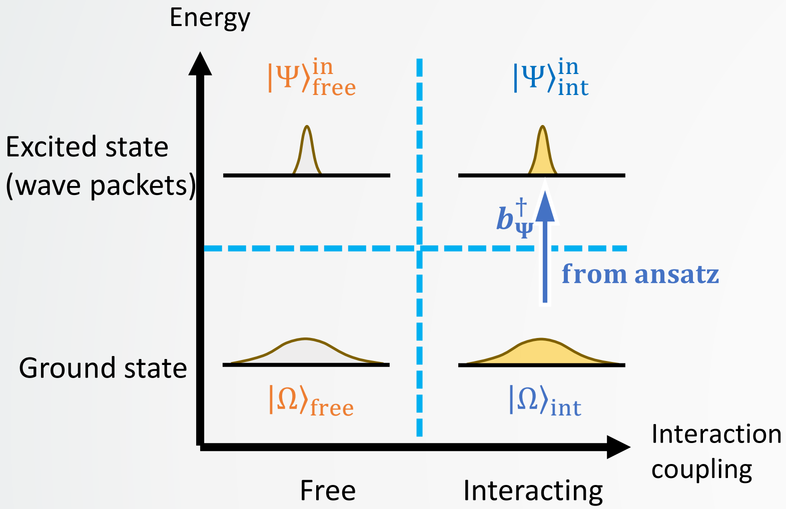

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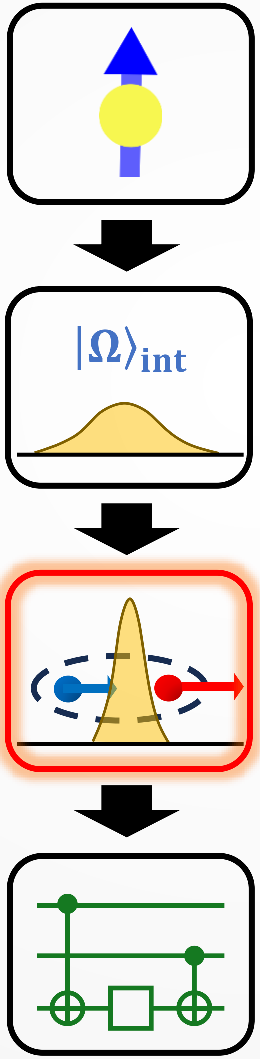
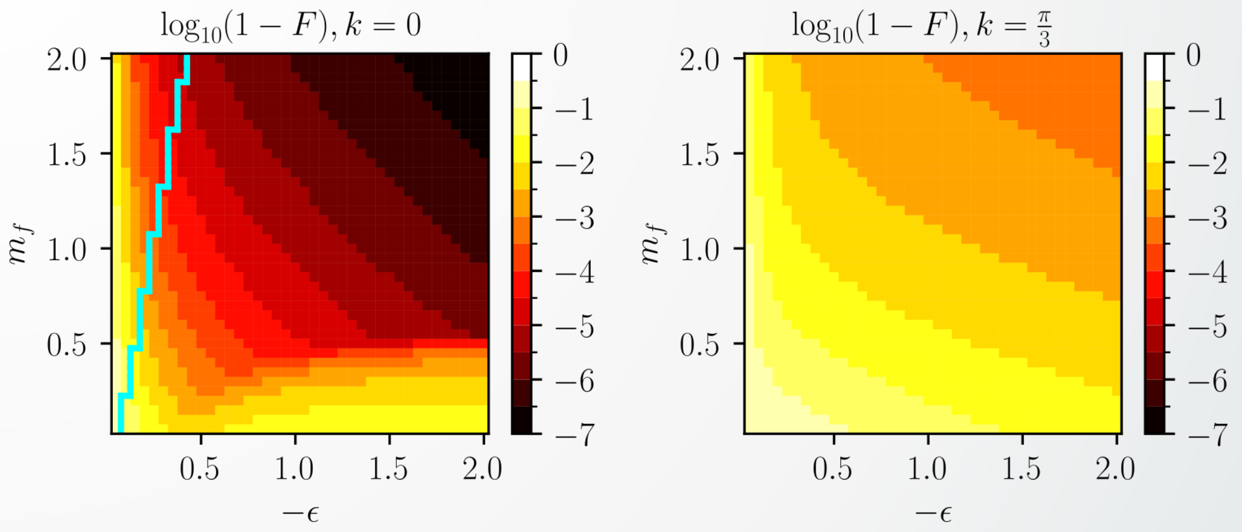
$$a = 1, N = 6$$

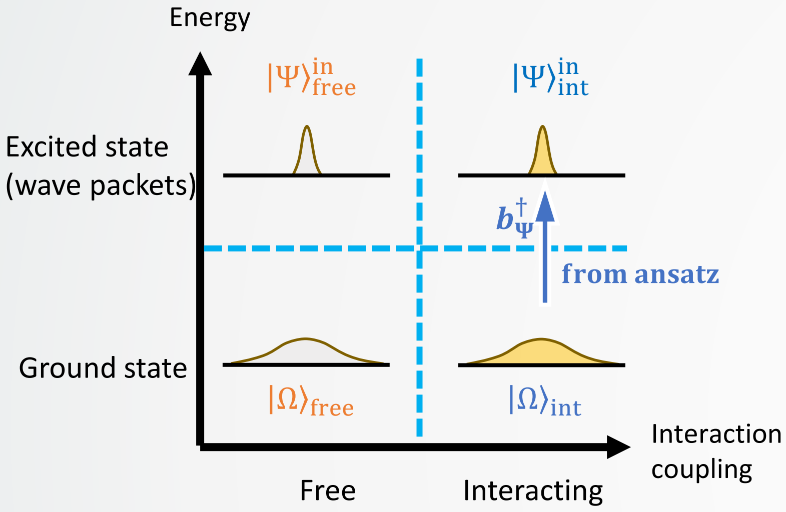


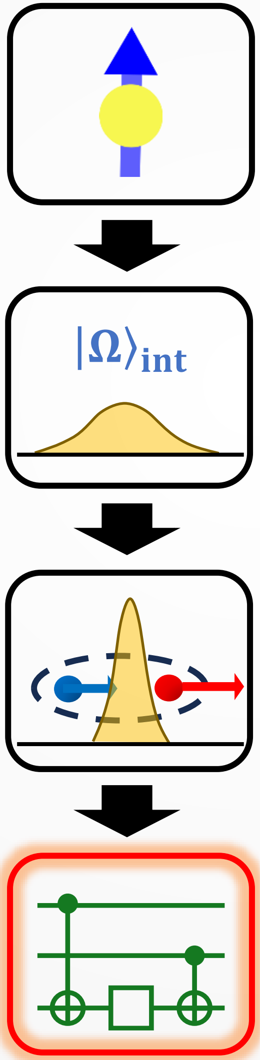
- **VQE** gives $|k\rangle$ (lowest energy other than ground state)
- Classical simulation of VQE in this work due to resource limit

For each momentum k: (6 sites)



Algorithm: quantum circuit





$$b^\dagger_{\boldsymbol{\Psi}} = \sum_k \Psi(k) b^\dagger_k = \sum_{m,n} \boldsymbol{C_{m,n}} \sigma^-_m \sigma^+_n \left(\prod_{l=m+1}^{n-1} \sigma^z_l \right) \left(\prod_{l=m}^{n-1} \tilde{\sigma}^x_l \right)$$

Optimized $(\boldsymbol{\mu^A_k}, \boldsymbol{\sigma^A_k})$

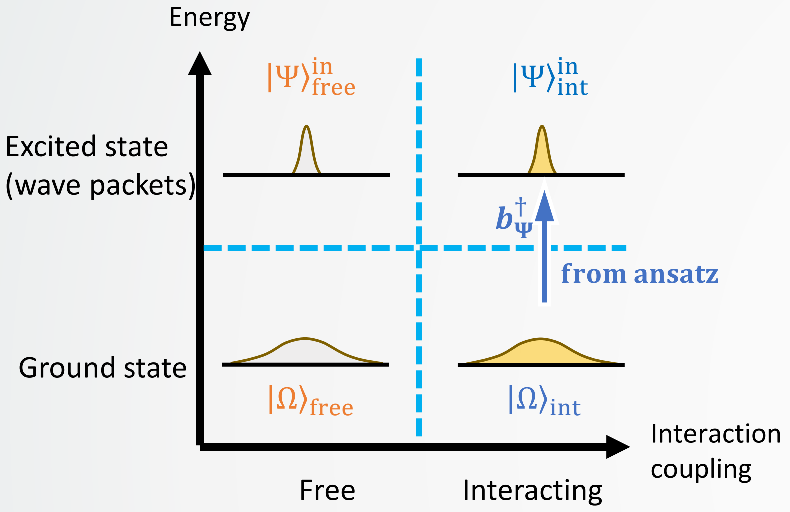
$\xi^\dagger_m \left(\prod_{l=m}^{n-1} \tilde{\sigma}^x_l \right) \xi_n$

1+1D Z_2 LGT coupled to fermions (PBC)

$$H = \frac{1}{2} \sum_{n=0}^{N-1} \left(\xi^\dagger_n \xi_{n+a} \tilde{\sigma}^x_n + \mathrm{H.c.} \right) + a m_f \sum_{n=0}^{N-1} (-1)^{\frac{n}{a}} \xi^\dagger_n \xi_n + a\epsilon \sum_{n=0}^{N-1} \tilde{\sigma}^z_n$$

$$a = 1, N = 6$$

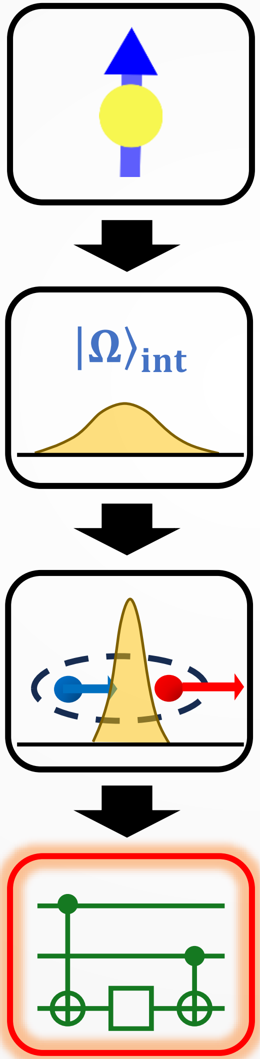
Algorithm: quantum circuit



1+1D Z_2 LGT coupled to fermions (PBC)

$$H = \frac{1}{2}\sum_{n=0}^{N-1}\left(\xi_n^\dagger \xi_{n+a}\tilde{\sigma}_n^x + \mathrm{H.c.}\right) + am_f\sum_{n=0}^{N-1}(-1)^{\frac{n}{a}}\xi_n^\dagger\xi_n + a\epsilon\sum_{n=0}^{N-1}\tilde{\sigma}_n^z$$

$$a = 1, N = 6$$



$$\boldsymbol{b}^\dagger_{\boldsymbol{\Psi}} = \sum_k \Psi(k) b_k^\dagger \quad = \sum_{m,n} \boldsymbol{C}_{\boldsymbol{m,n}} \sigma_m^- \sigma_n^+ \left(\prod_{l=m+1}^{n-1} \sigma_l^z\right)\left(\prod_{l=m}^{n-1} \tilde{\sigma}_l^x\right)$$

Optimized$(\boldsymbol{\mu}_{\boldsymbol{k}}^{\boldsymbol{A}}, \boldsymbol{\sigma}_{\boldsymbol{k}}^{\boldsymbol{A}})$ $\quad \xi_m^\dagger\left(\prod_{l=m}^{n-1}\tilde{\sigma}_l^x\right)\xi_n$

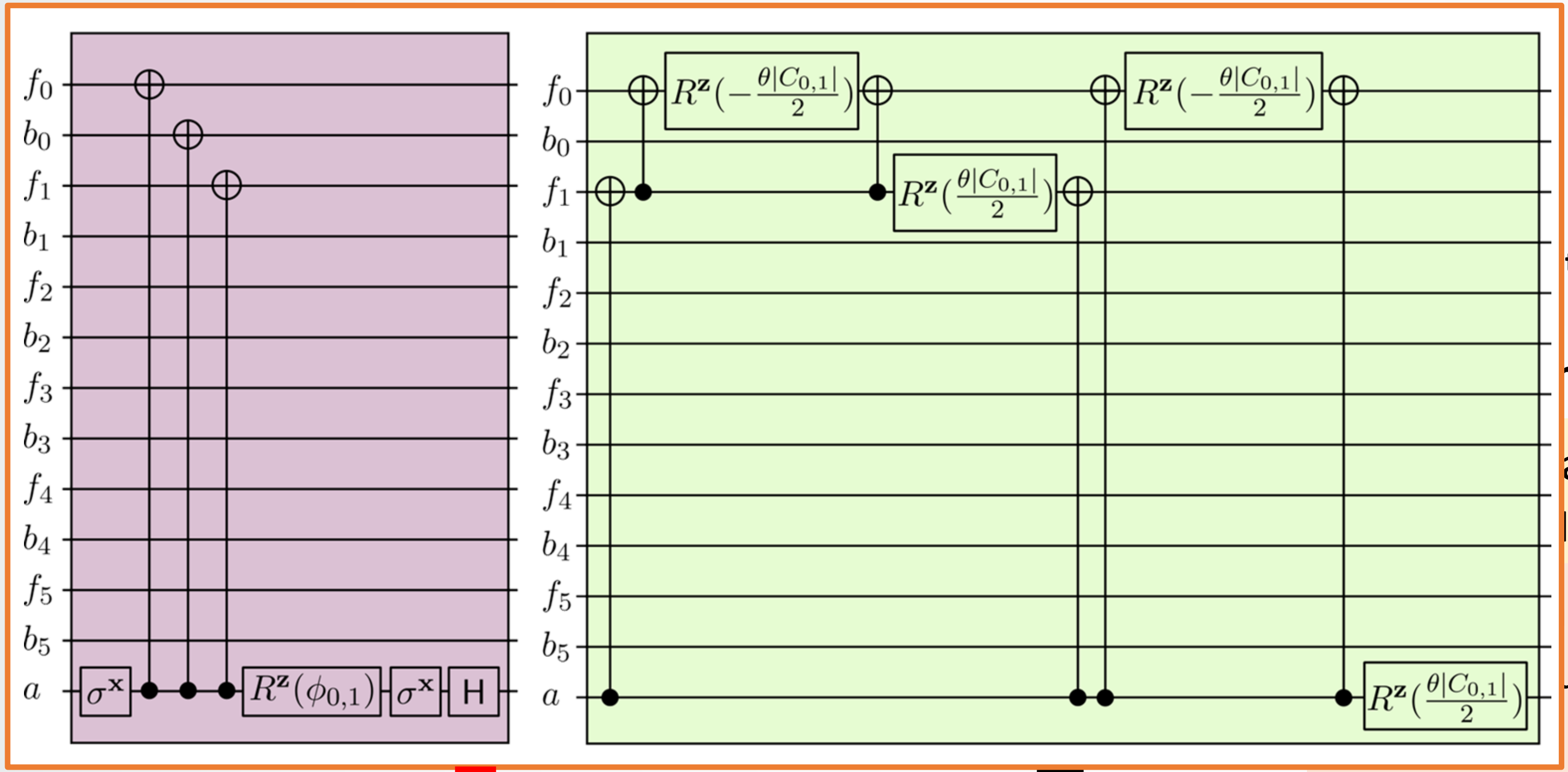
Technical issues and solutions

- Non-unitary operator $b^\dagger_\Psi$
  - Ancilla encoding
- Non-commuting summands in $b^\dagger_\Psi$
  - Product formula (Trotterization)

    $$e^{A+B} = \lim_{n\to\infty}\left(e^{A/n}e^{B/n}\right)^n$$
- Complicated multi-spin operator
  - Choose a better basis using Singular Value Decomposition (SVD) circuit

Z. Davoudi, A. F. Shaw, J. R. Stryker, Quantum 7, 1213 (2023)

Algorithm: quantum circuit



$$= \sum_{m,n} \boldsymbol{C_{m,n}} \sigma_m^- \sigma_n^+ \left(\prod_{l=m+1}^{n-1} \sigma_l^z\right)\left(\prod_{l=m}^{n-1} \tilde{\sigma}_l^x\right)$$

timized$(\boldsymbol{\mu_k^A}, \boldsymbol{\sigma_k^A})$ $\xi_m^\dagger\left(\prod_{l=m}^{n-1} \tilde{\sigma}_l^x\right)\xi_n$

nical issues and solutions

ary operator $b_\Psi^\dagger$

la encoding

muting summands in $b_\Psi^\dagger$

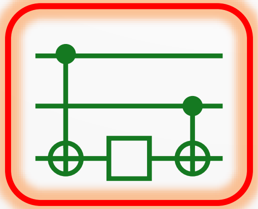
uct formula (Trotterization)

$= \lim_{n\to\infty}\left(e^{A/n}e^{B/n}\right)^n$

- Complicated multi-spin operator
  - Choose a better basis using Singular Value Decomposition (SVD) circuit

# of gates polynomial in system size

Realize on hardware!



Z. Davoudi, A. F. Shaw, J. R. Stryker, Quantum 7, 1213 (2023)

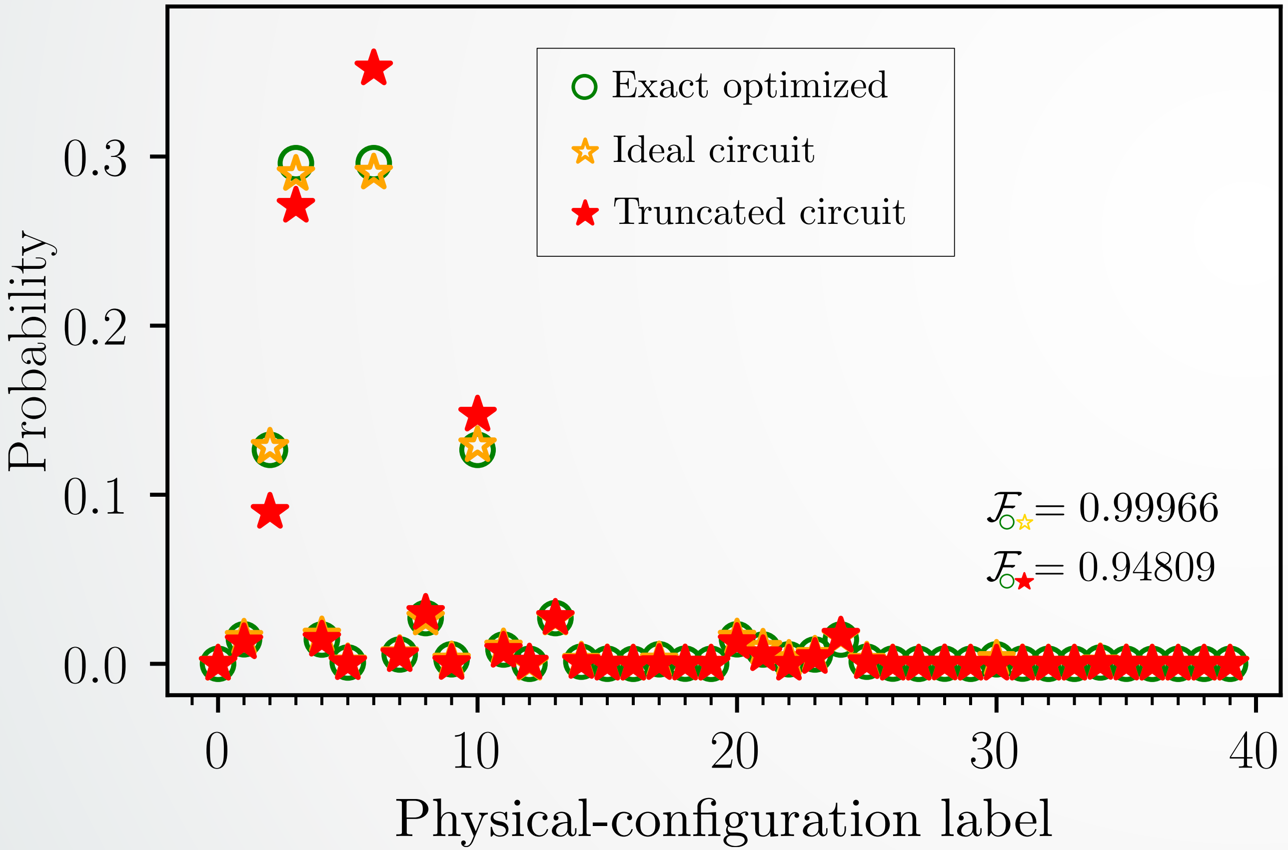
Results: Quantinuum H1-1

Z_2 wavepacket results

$$\Psi(k) = \mathcal{N}_\Psi \exp(-ik\mu) \exp\left(\frac{-(k-k_0)^2}{4\sigma}\right)$$

6 sites (12 + 1 qubits), $m_f = 1, \epsilon = -0.3$

$$\sigma = \frac{\pi}{6}, \mu = 3, k_0 = 0$$



- **Exact optimized:**
  Assemble the optimized $|k\rangle$ classically according to the wave packet profile $\Psi(k)$
- **Ideal circuit:**
  Fine steps in product formula
- **Truncated circuit:**
  Crude steps in product formula, only keep "important" mesons ($|C_{m,n}| > 0.1$)

Z_2 wavepacket results

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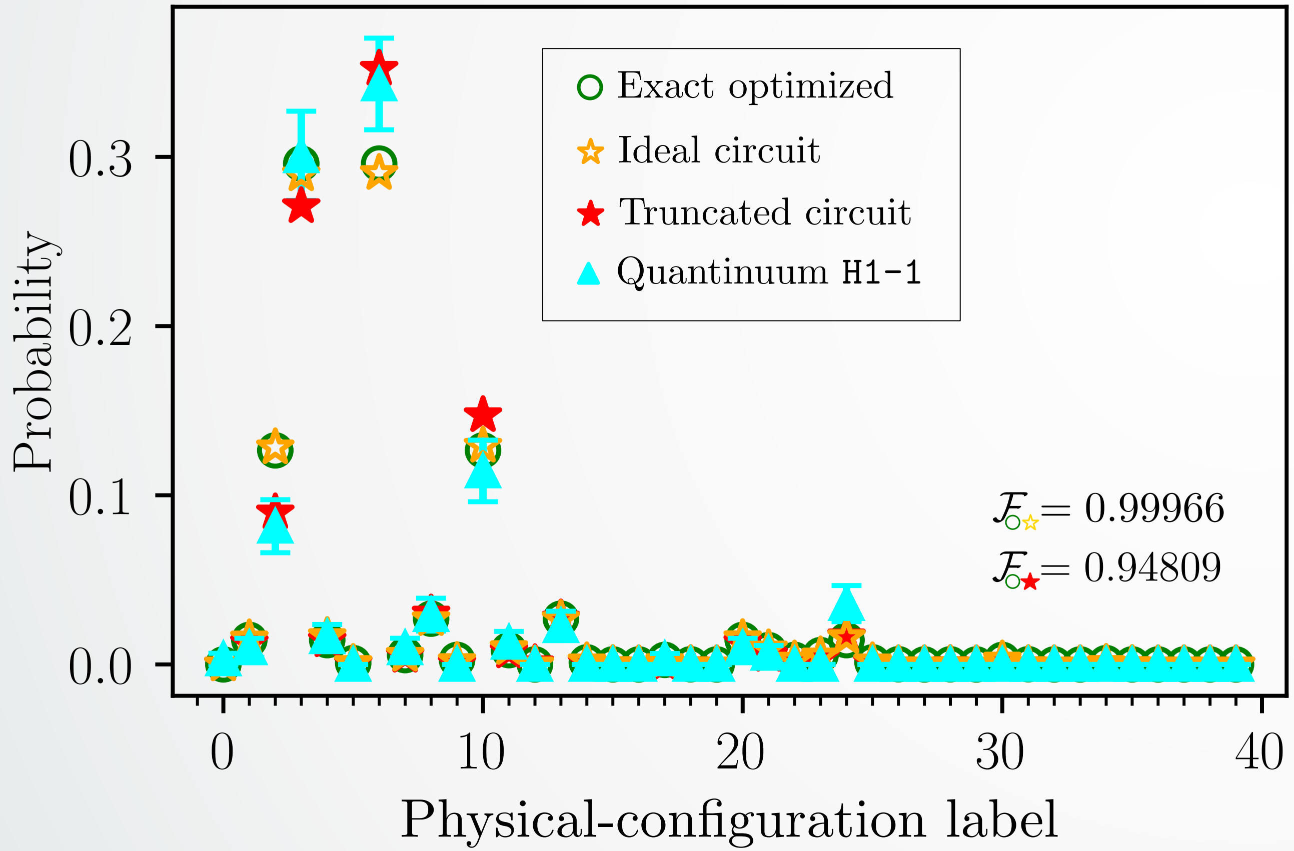

- **Exact optimized:**
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  Fine steps in product formula
- **Truncated circuit:**
  Crude steps in product formula, only keep "important" mesons ($|C_{m,n}| > 0.1$)
- **Quantinuum H1-1:**
  500 shots on truncated circuit

QUANTINUUM

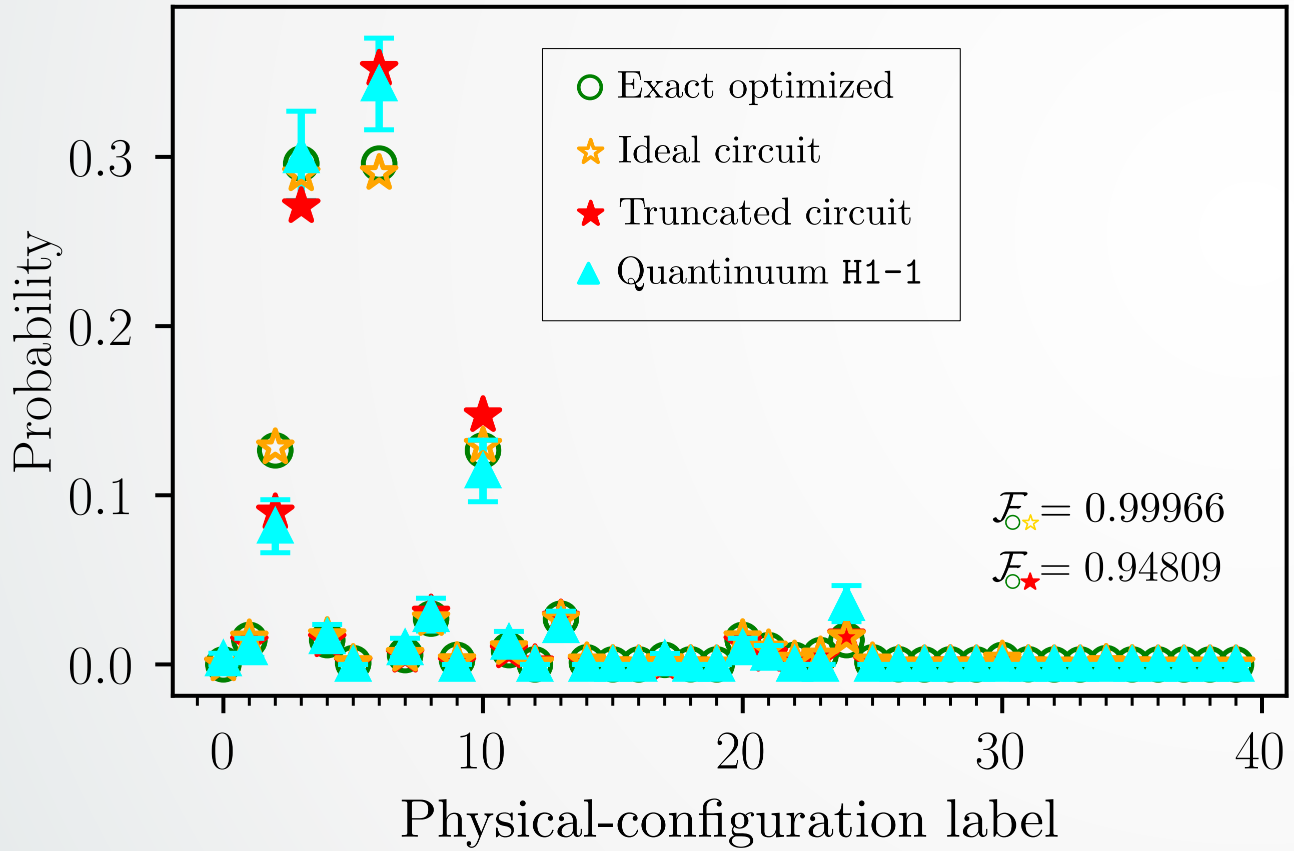
✓ Trapped ion with 20 qubits
✓ all-to-all connectivity
✓ $\sim 10^{-5}$ single-qubit gate infidelity
✓ $\sim 10^{-3}$ two-qubit gate infidelity

Z_2 wavepacket results

$$\boldsymbol{\Psi}(\boldsymbol{k}) = \mathcal{N}_\Psi \exp(-ik\boldsymbol{\mu}) \exp\left(\frac{-(k-\boldsymbol{k_0})^2}{4\boldsymbol{\sigma}}\right)$$

6 sites (12 + 1 qubits), $m_f = 1, \epsilon = -0.3$

$$\boldsymbol{\sigma} = \frac{\boldsymbol{\pi}}{\mathbf{6}}, \boldsymbol{\mu} = \mathbf{3}, \boldsymbol{k_0} = \mathbf{0}$$



- **Exact optimized:**
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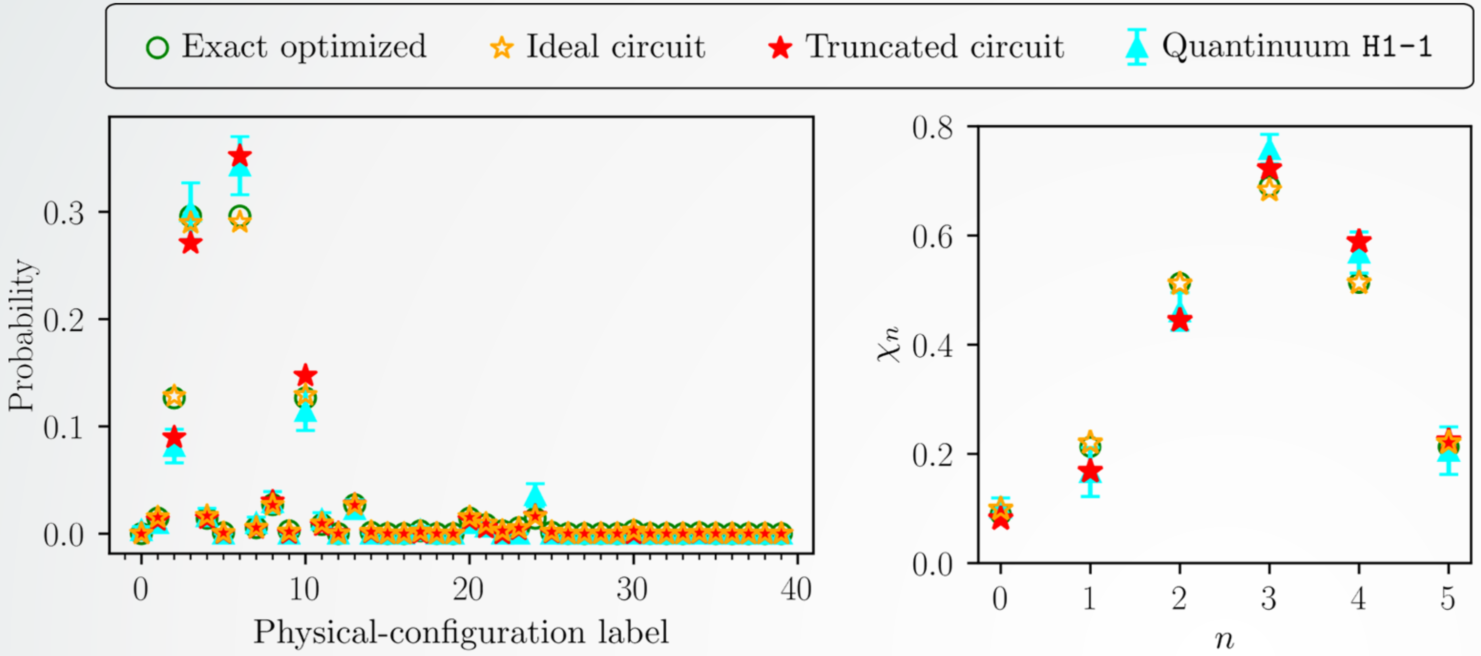
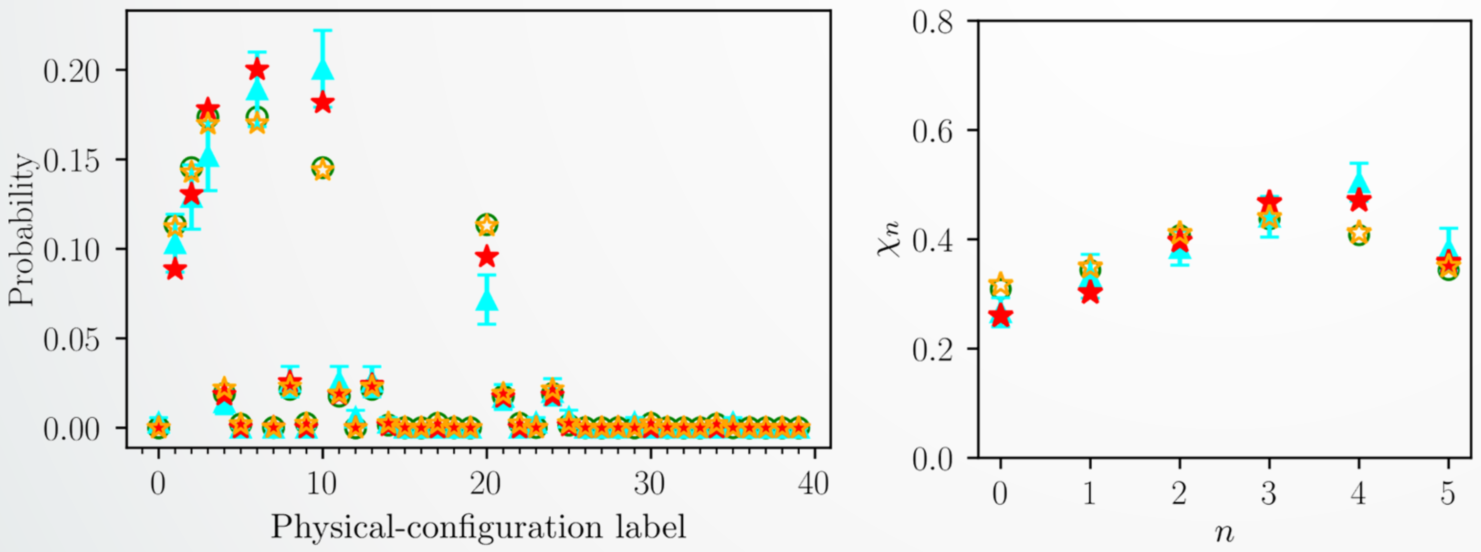
- **Truncated circuit:**
  Crude steps in product formula, only keep "important" mesons ($|C_{m,n}| > 0.1$)
- **Quantinuum H1-1:**
  500 shots on truncated circuit

Symmetry-based error mitigation
- Probability leakage to non-physical Hilbert space due to noise
- Only count the physical outcome



(a) Wave packet with $\sigma = \frac{\pi}{6}$, $\mu = 3$, and $k_0 = 0$



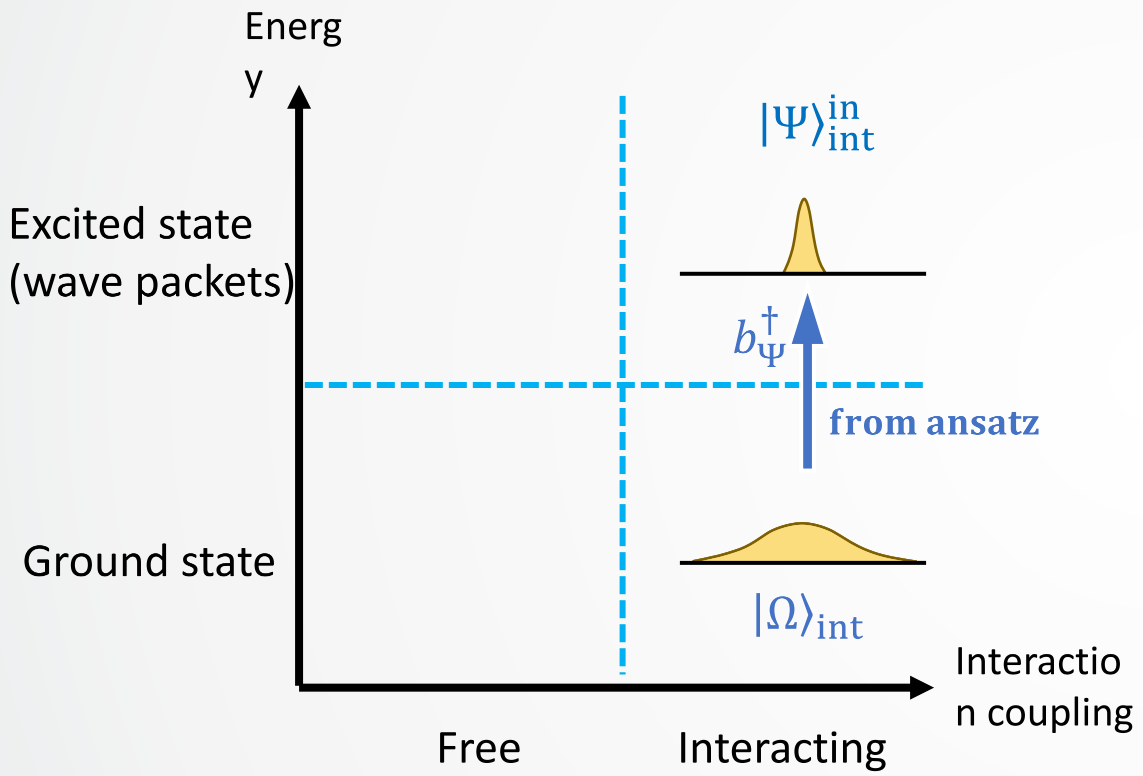
(b) Wave packet with $\sigma = \frac{\pi}{10}$, $\mu = 3$, and $k_0 = 0$

	$\sigma = \frac{\pi}{6}$	$\sigma = \frac{\pi}{10}$
# of CNOT gates	308	180
Physical events	306/500	349/500

- Staggered density:

$$\chi_n = \begin{cases} \langle \Psi | \xi_n^\dagger \xi_n | \Psi \rangle, n \in even \\ 1 - \langle \Psi | \xi_n^\dagger \xi_n | \Psi \rangle, n \in odd \end{cases}$$

Summary & outlook



- **Goal: to alleviate the state preparation bottleneck**
- **Efficient way to build interacting wave packets:**
  - Mesonic ansatz
  - Quantum algorithm
  - Efficient circuits realizable on hardware
- **Hardware results (Quantinuum):**
  - Good agreement with classical computation
  - Simple (symmetry-based) error mitigation

- **Outlook**
  - Other hadronic ansatz, non-abelian gauge theory…
  - **Prepare 2 wave packets and perform scattering**

Thanks for listening!

Appendix

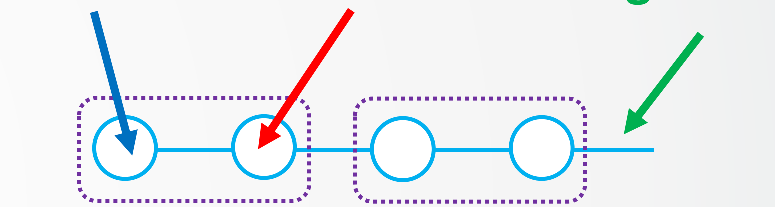
1+1D LGTs coupled to staggered fermions

- Hamiltonian:

$a = 1$

$$H = \underbrace{\frac{1}{2}\sum_n \left(\xi_n^\dagger \xi_{n+a} U_n + \text{H.c.}\right)}_{H^h} + \underbrace{a m_f \sum_n (-1)^{\frac{n}{a}} \xi_n^\dagger \xi_n}_{H^m} + \underbrace{a\epsilon \sum_n f(E_n)}_{H^\epsilon}$$

Staggered formulation

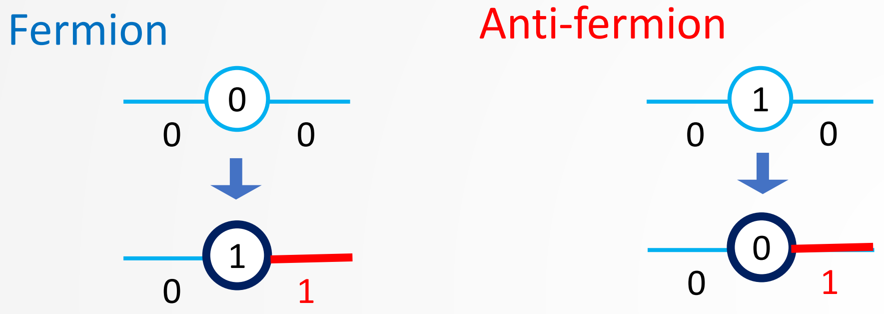


Theory	$f(E_n)$	U	E	Gauss' law: $G_n\lvert\psi_{phys}\rangle = g\lvert\psi_{phys}\rangle, \forall n$
Z_2	E_n	$\tilde{\sigma}^x$	$\tilde{\sigma}^z$	$G_n = E_n E_{n-1} \exp\left(i\pi\left(\xi_n^\dagger \xi_n - \frac{1-(-1)^n}{2}\right)\right), g = 1$
$U(1)$	E_n^2	$\Sigma_l \lvert l+1\rangle\langle l\rvert$	$\Sigma_l l \lvert l\rangle\langle l\rvert$	$G_n = E_n - E_{n-1} + \xi_n^\dagger \xi_n - \frac{1-(-1)^n}{2}, g = 0$

$l \in \mathbb{Z} \to |l| \leq \Lambda$

1+1D LGTs coupled to staggered fermions (Z_2)

- Gauss' law for Z_2



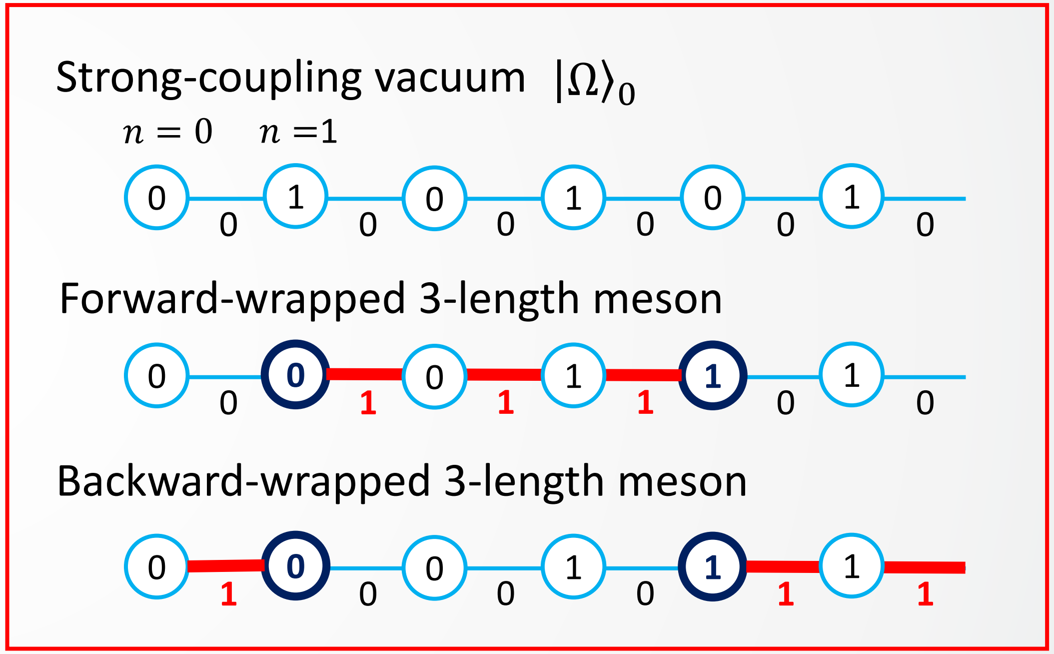
- PBC:
  - Well-defined momentum states

$$k \in \tilde{\Gamma} = \frac{2\pi}{N}\left\{-\frac{N}{2}, -\frac{N}{2}+1, \cdots, \frac{N}{2}-1\right\} \cap \left[-\frac{\pi}{2}, \frac{\pi}{2}\right)$$

- Mapping to qubits

Jordan-Wigner: $\begin{cases} \xi_n^\dagger = \left(\prod_{j<n} \sigma_j^z\right)\sigma_n^- \\ \xi_n = \left(\prod_{j<n} \sigma_j^z\right)\sigma_n^+ \end{cases}$

Physical Hilbert space



$$H = \frac{1}{2}\sum_n (\sigma_n^- \sigma_{n+1}^+ \tilde{\sigma}_n^x + \mathrm{H.c.}) + m_f \sum_n (-1)^n \sigma_n^- \sigma_n^+ + \epsilon \sum_n \tilde{\sigma}_n^z$$

- Hopping on the boundary: $\sigma_{n-1}^- \sigma_0^+ \tilde{\sigma}_{n-1}^x (-1)^{\Sigma_n \xi_n^\dagger \xi_n + 1}$

Ansatz for creation operator

$$b_k^\dagger = \sum_{p,q\in\tilde{\Gamma}} \delta_{k-p-q}\,\eta(p,q)\,\mathcal{B}(p,q)$$

Conservation of momentum — Ansatz — Mesonic creation operator

$$\boldsymbol{\eta(p,q)} = N_\eta \exp\left(\frac{i(p-q)\boldsymbol{\mu_k^A}}{2}\right)\exp\left(\frac{-(p-q)^2}{4\boldsymbol{\sigma_k^A}^{\mathbf{2}}}\right)$$

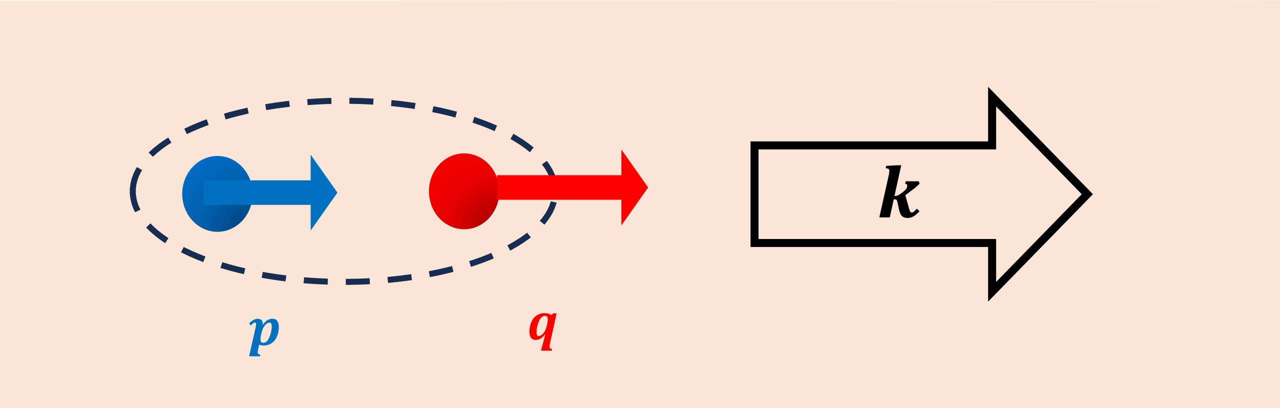
$$\mathcal{B}(p,q) = \sum_{m,n\in\Gamma} \mathcal{C}(p,m)\mathcal{D}(q,n)\mathcal{M}_{m,n}$$

$$\mathcal{C}(p,m) = \sqrt{\frac{m_f+\omega_p}{2\pi\omega_p}}\left[\mathcal{P}_{m0}+v_p\mathcal{P}_{m1}\right]e^{ipm} \quad \mathcal{D}(q,n) = \sqrt{\frac{m_f+\omega_q}{2\pi\omega_q}}\left[-v_q\mathcal{P}_{n0}+\mathcal{P}_{n1}\right]e^{iqn}$$

$$\boldsymbol{\mathcal{M}_{m,n}} = \boldsymbol{\xi_m^\dagger}\left(\prod_{l=m}^{n-1}\boldsymbol{U_l}\right)\boldsymbol{\xi_n}\ or\ \boldsymbol{\xi_m^\dagger}\left(\prod_{l=m-1}^{0}\boldsymbol{U_l^\dagger}\right)\left(\prod_{l=N-1}^{n}\boldsymbol{U_l^\dagger}\right)\boldsymbol{\xi_n}$$

In each k sector:

- **Optimize** for lowest energy
  $\langle\Omega|b_k(\mu_k^A,\sigma_k^A)|H|b_k^\dagger(\mu_k^A,\sigma_k^A)|\Omega\rangle$
- Obtain the variables
  $b_k^\dagger(\boldsymbol{\mu_k^{A*}},\boldsymbol{\sigma_k^{A*}})|\Omega\rangle = |\mathrm{k}\rangle$



Ansatz for creation operator

$$\boldsymbol{\Psi(k)} = \mathcal{N}_\Psi \exp(-ik\boldsymbol{\mu}) \exp\left(\frac{-(k-\boldsymbol{k_0})^2}{4\boldsymbol{\sigma}}\right)$$

Adopted

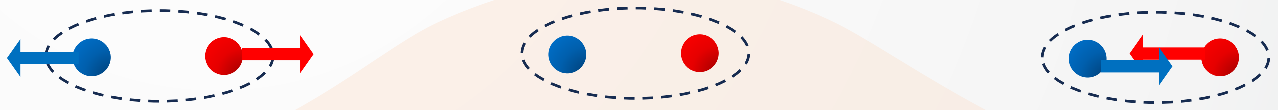
$$\boldsymbol{b_\Psi^\dagger} = \sum_k \Psi(k) b_k^\dagger$$

$$\Psi\left(k=-\frac{\pi}{3}\right)\cdot b^\dagger_{k=-\frac{\pi}{3}} \qquad \Psi(k=0)\cdot b^\dagger_{k=0} \qquad \Psi\left(k=\frac{\pi}{3}\right)\cdot b^\dagger_{k=\frac{\pi}{3}}$$

$$\boldsymbol{\eta(p,q)} = N_\eta \exp\left(\frac{i(p-q)\boldsymbol{\mu_k^A}}{2}\right)\exp\left(\frac{-(p-q)^2}{4\boldsymbol{\sigma_k^A}^2}\right)$$

Optimized

$$\eta\left(-\frac{\pi}{3},\frac{\pi}{3}\right)\mathcal{B}\left(-\frac{\pi}{3},\frac{\pi}{3}\right) \qquad \eta(0,0)\mathcal{B}(0,0) \qquad \eta\left(\frac{\pi}{3},-\frac{\pi}{3}\right)\mathcal{B}\left(\frac{\pi}{3},-\frac{\pi}{3}\right)$$

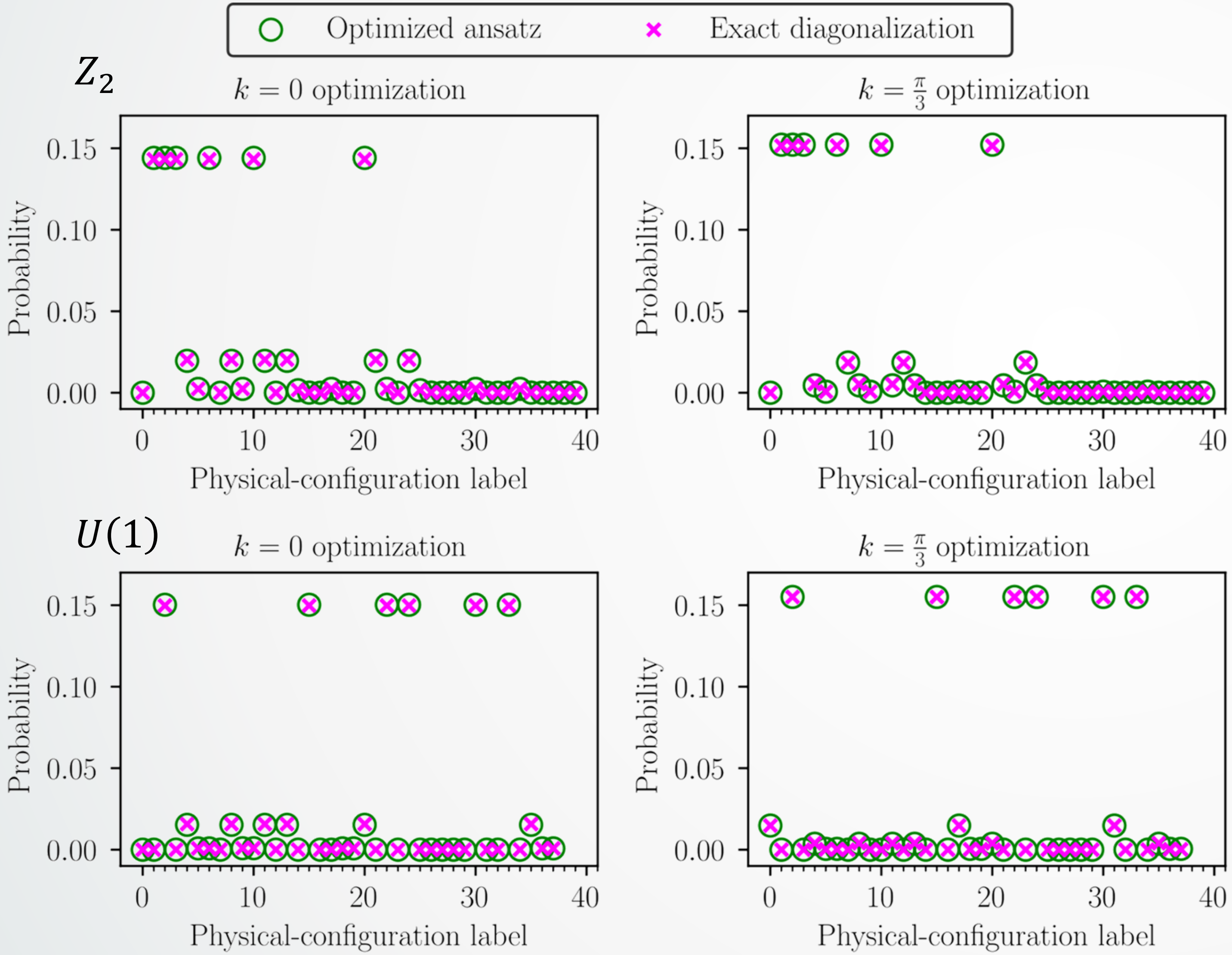


$$\boldsymbol{p=-\frac{\pi}{3}, q=\frac{\pi}{3}} \qquad \boldsymbol{p=0, q=0} \qquad \boldsymbol{p=\frac{\pi}{3}, q=-\frac{\pi}{3}}$$

$$b_\Psi^\dagger = \sum_{m,n} C_{m,n}\widetilde{\mathcal{M}}_{m,n}$$

$$C_{m,n} = \sum_k \boldsymbol{\Psi(k)} \sum_{p,q\in\tilde{\Gamma}} \delta_{k-p-q}\boldsymbol{\eta(p,q)} \sqrt{\frac{m_f+\omega_p}{2\pi\omega_p}}\sqrt{\frac{m_f+\omega_q}{2\pi\omega_q}}\left[\mathcal{P}_{m0}+v_p\mathcal{P}_{m1}\right]\left[-v_q\mathcal{P}_{n0}+\mathcal{P}_{n1}\right]e^{i(pm+qn)}$$

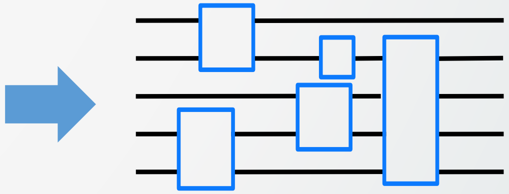
k-momentum state amplitude (6 sites)

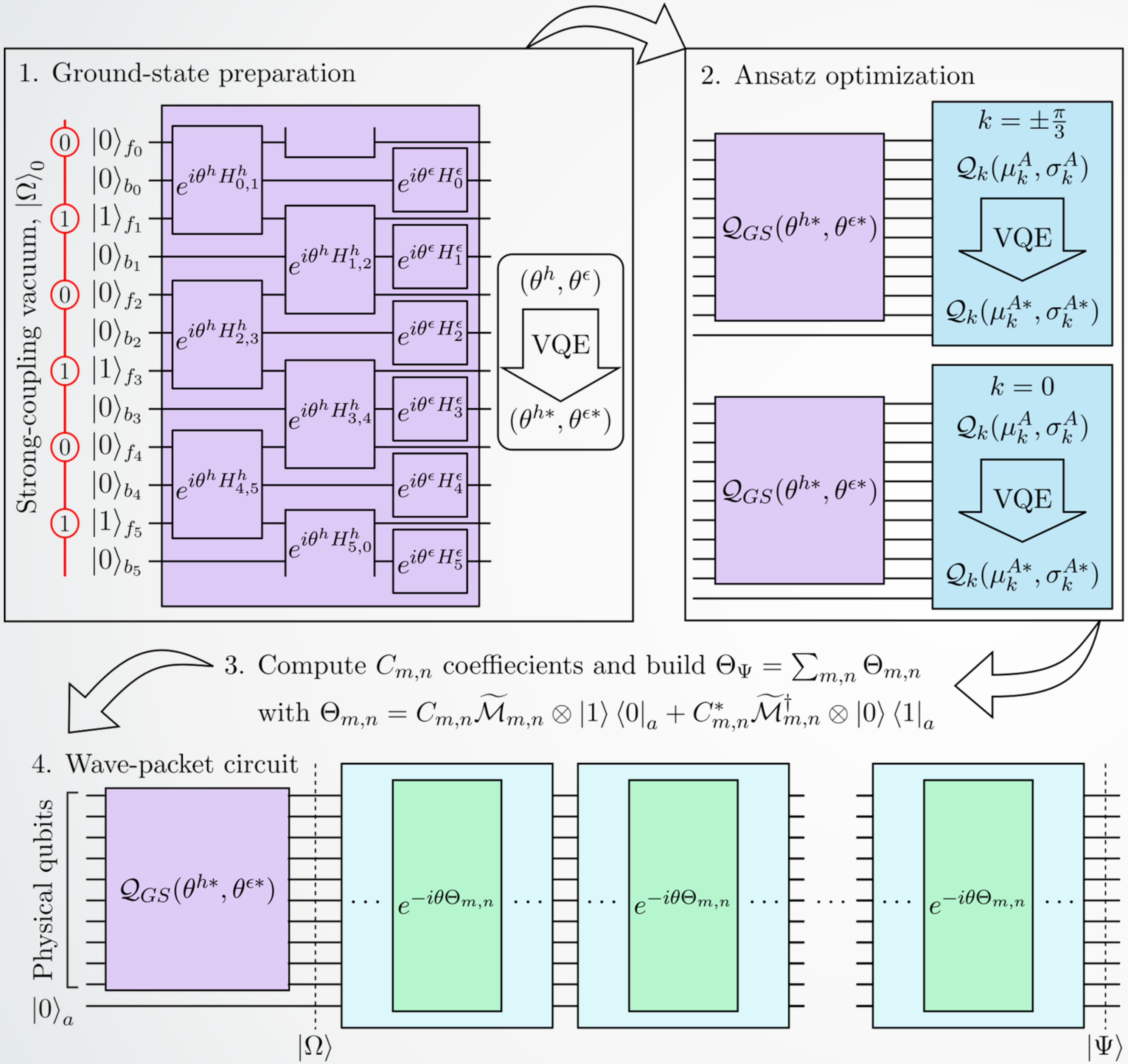


	k	$1 - F$	$\delta E \equiv \frac{\lvert E_{exact} - E_{opt} \rvert}{\lvert E_{exact} \rvert}$
Z_2, $m = 1.0$, $\epsilon = -0.3$	0	2.27×10^{-4}	2.03×10^{-4}
	$\frac{\pi}{3}$	1.24×10^{-2}	4.24×10^{-3}
$U(1)$, $m = 1.0$, $\epsilon = 1.0$	0	5.38×10^{-5}	5.50×10^{-4}
	$\frac{\pi}{3}$	7.79×10^{-3}	3.93×10^{-2}

- Optimization doable and verified with VQE using exact state evolution. For efficiency, currently done classically.

$$\boldsymbol{b}_{\boldsymbol{\Psi}}^{\dagger} |\boldsymbol{\Omega}\rangle = |\boldsymbol{\Psi}\rangle$$

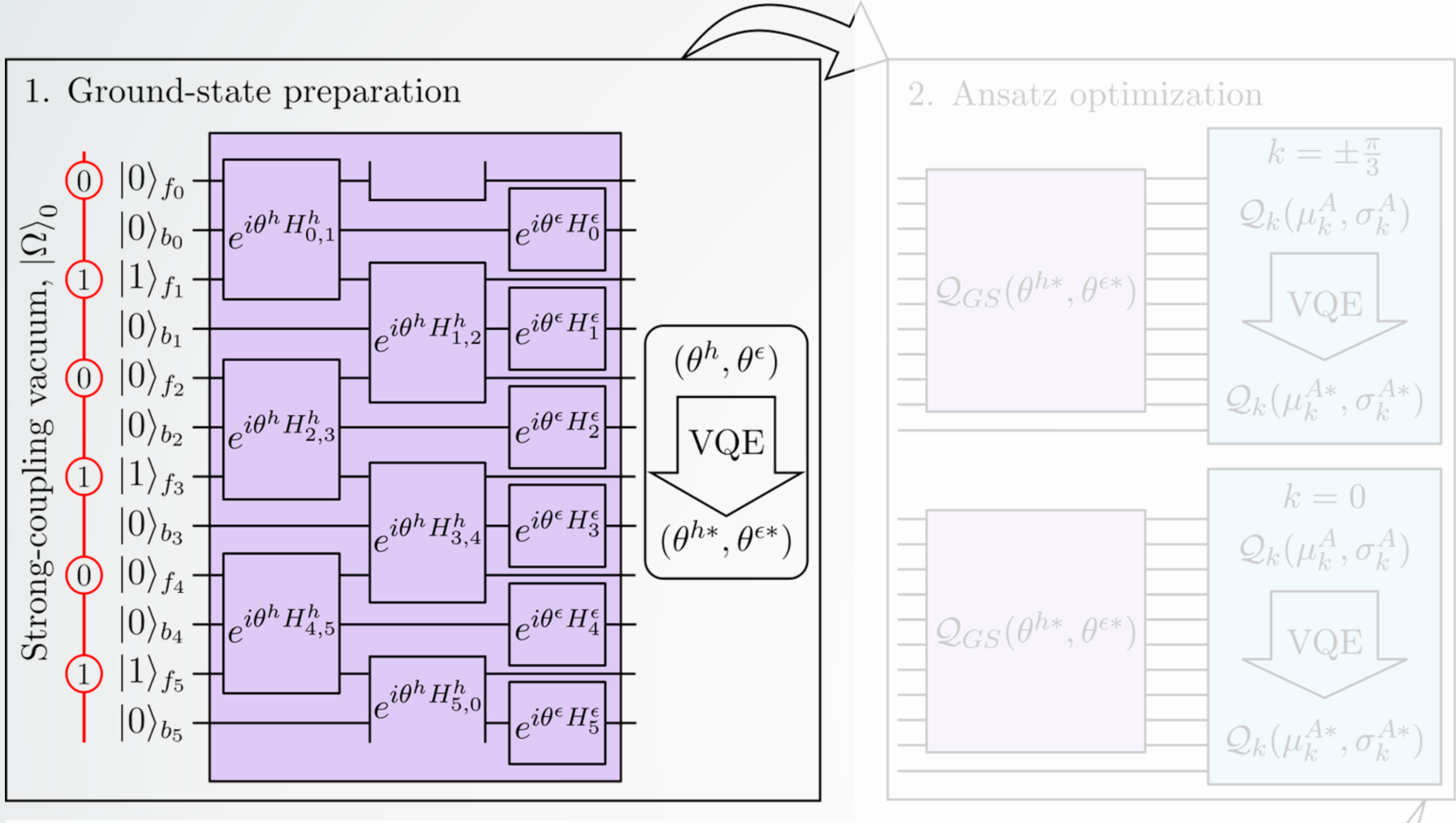




Algorithm

- 6-site Z_2 theory
- 40 physical configurations
- $k \in \left[-\frac{\pi}{3}, 0, \frac{\pi}{3}\right]$
- $m_f = 1, \epsilon = -0.3$

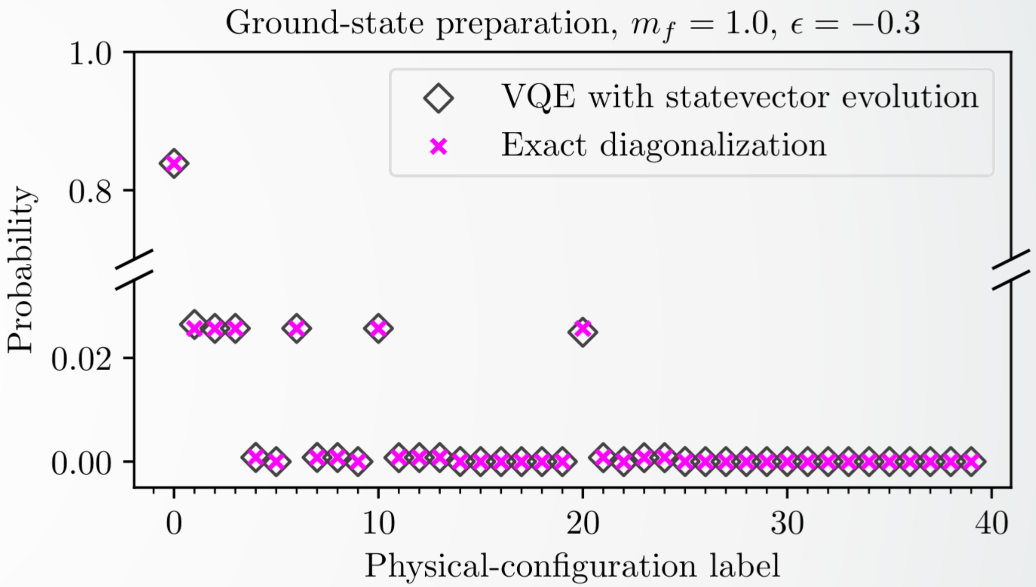
Ground state preparation



$$|\Omega\rangle = \mathcal{Q}_{GS}|\Omega_0\rangle$$

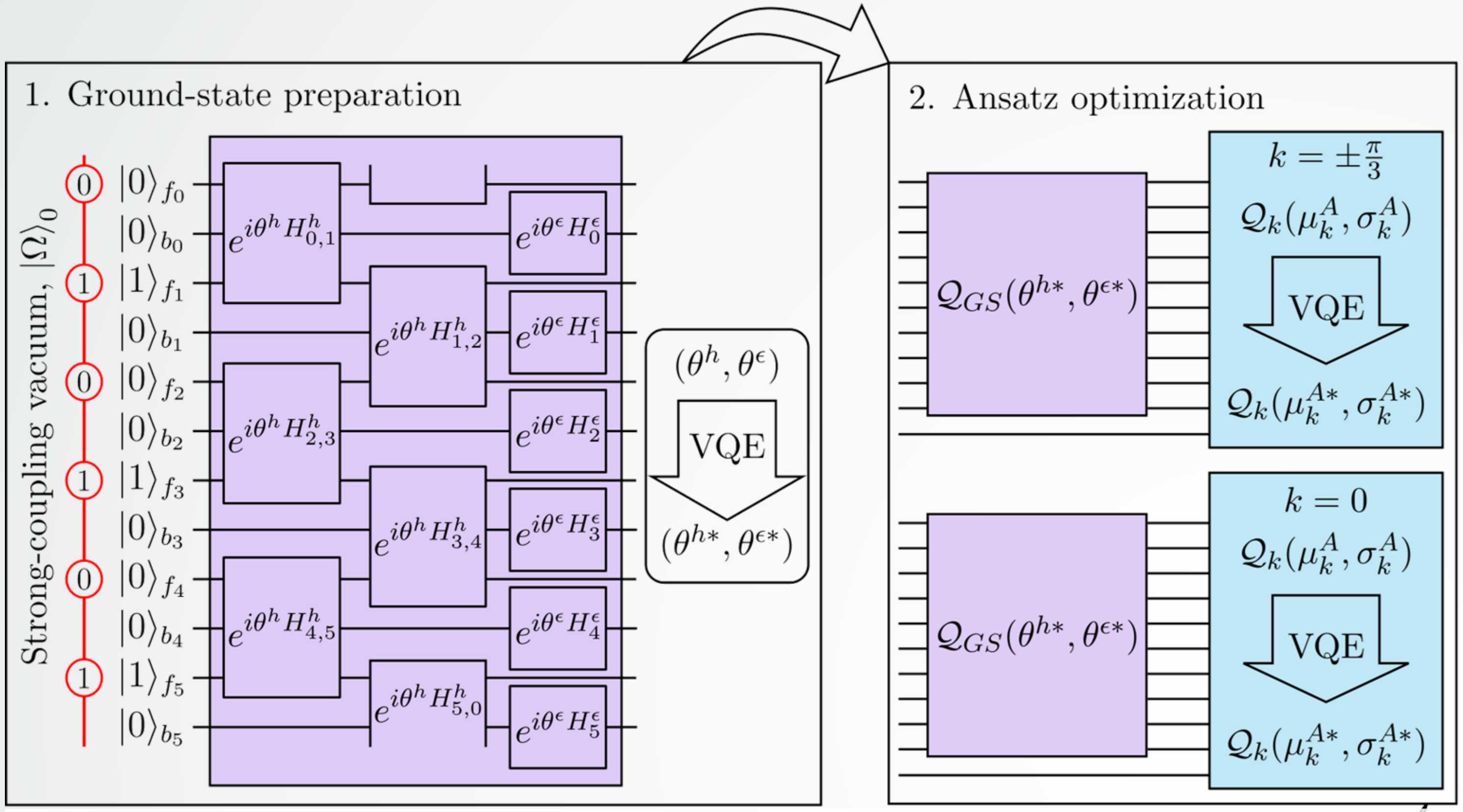
$$\mathcal{Q}_{GS} = \prod_{j=1}^{N_{GS}} \left(\prod_n e^{i\theta_j^h H_{n,n+1}^h} \right) \left(\prod_n e^{i\theta_j^m H_n^m} \right) \left(\prod_n e^{i\theta_j^\epsilon H_n^\epsilon} \right)$$

$N_{GS} = 1$, parameters: $\theta^h, \theta^\epsilon$



$$1 - F_{GS} = 7.83 \times 10^{-5}$$

- **VQE inspiration**
  L. Lumia, P. Torta, G. B. Mbeng, G. E. Santoro, E. Ercolessi, M. Burrello, and M. M. Wauters, PRX Quantum 3, 020320
- **Scalable Adapt-VQE**
  R. C. Farrell, M. Illa, A. N. Ciavarella, M. J. Savage, PRX Quantum 5 (2024) 2, 020315



	VQE on quantum computer	VQE classical simulation with exact statevector	Classical optimiz-ation in physical Hilbert space
GS preparation	✗	✓	
k-momentum	✗	✓	Parameter scan

Optimization and after

$$b_\Psi^\dagger = \sum_{m,n} C_{m,n} \widetilde{\mathcal{M}}_{m,n}$$

$$= \sum_{m,n} C_{m,n} \sigma_m^- \sigma_n^+ \left(\prod_{l=m+1}^{n-1} \sigma_l^z \right) \left(\prod_{l=m}^{n-1} \tilde{\sigma}_l^x \right)$$

Issues:

- Non-unitary operator $b_\Psi^\dagger$
- Multi-spin operator, need efficient circuit design

Ancilla encoding & SVD circuit

Wave-packet circuit

- **Ancilla encoding** for non-unitary operators

$$b_\Psi^\dagger|\Omega\rangle = |\Psi\rangle \qquad [b_\Psi, b_\Psi^\dagger] = \mathbb{I}$$

$$\Theta \equiv b_\Psi^\dagger \otimes \mathbf{|1\rangle\langle 0|_a} + b_\Psi \otimes \mathbf{|0\rangle\langle 1|_a}$$

$$e^{-i\frac{\pi}{2}\Theta}|\Omega\rangle \otimes |0\rangle_a = -i|\Psi\rangle \otimes |1\rangle_a$$

  - For composite operator $\Theta = \Sigma_i \Theta_i$, requires Trotterization if summands don't commute

$$\Theta_{m,n} = \sum_{m,n} C_{m,n}\widetilde{\mathcal{M}}_{m,n} \otimes |1\rangle\langle 0|_a + C^*_{m,n}\widetilde{\mathcal{M}}^\dagger_{m,n} \otimes |0\rangle\langle 1|_a$$

S. P. Jordan, K. S. M. Lee, and J. Preskill, Quantum algorithms for quantum field theories, Science 336, 1130 (2012)

- **Singular Value Decomposition circuit**
  - Find a basis that diagonalizes

$$\Theta \equiv b_\Psi^\dagger \otimes |1\rangle\langle 0|_a + b_\Psi \otimes |0\rangle\langle 1|_a$$

$$\downarrow$$

$$b_\Psi^2 = {b_\Psi^\dagger}^2 = 0, b_\Psi = VSW^\dagger$$

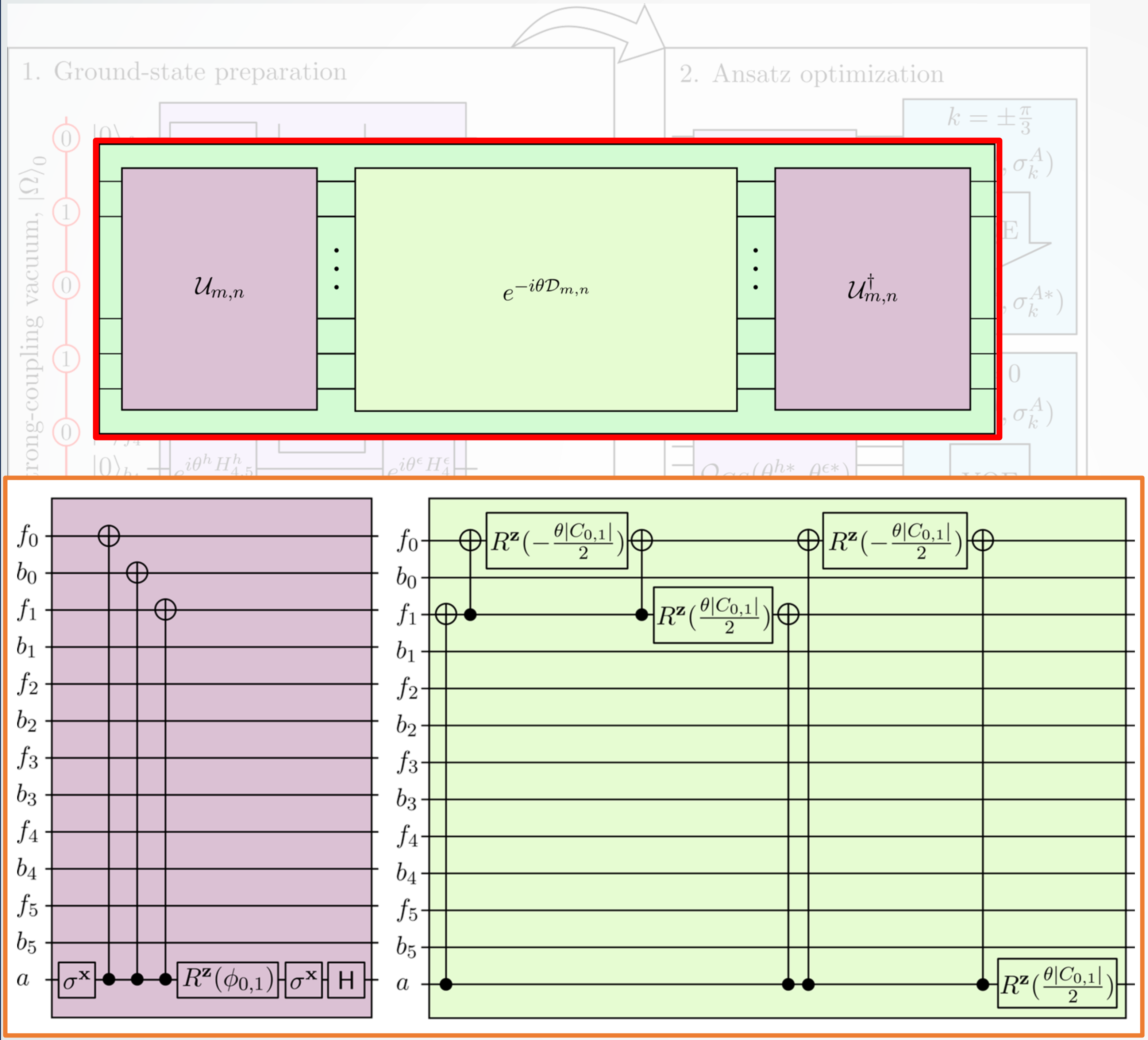
Suppose the SVD for b_Ψ is easy to obtain

$$\Theta = \mathcal{U}^\dagger D \mathcal{U}$$

$$\begin{cases} \mathcal{U} = (\mathrm{Had}_a)\left(V^\dagger \otimes |0\rangle\langle 0|_a + W^\dagger \otimes |1\rangle\langle 1|_a\right) \\ D = S \otimes \sigma_a^z \end{cases}$$

$$\boldsymbol{e^{-i\frac{\pi}{2}\Theta_{m,n}} = \mathcal{U}^\dagger_{m,n} e^{-i\frac{\pi}{2}D_{m,n}} \mathcal{U}_{m,n}}$$

Z. Davoudi, A. F. Shaw, J. R. Stryker, Quantum 7, 1213 (2023)



Ground state preparation

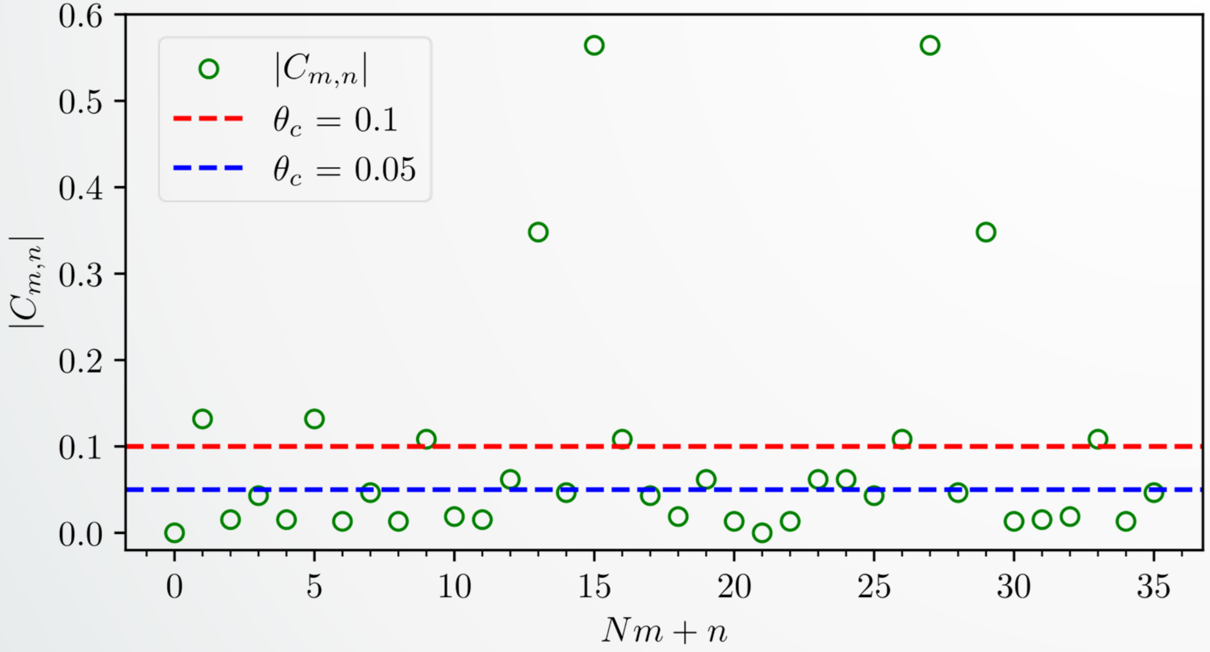
$$e^{-i\frac{\pi}{2}\Theta_{m,n}} = \mathcal{U}^\dagger_{m,n} e^{-i\frac{\pi}{2}D_{m,n}} \mathcal{U}_{m,n}$$

$$\begin{cases} C_{m,n} = |C_{m,n}| e^{i\phi_{m,n}} \\ V_{m,n} = e^{\frac{-i\phi_{m,n}}{2}} \sigma^z_m \sigma^z_n \left(\prod_{l=m}^{n-1} \tilde{\sigma}^X_l \right) \\ W_{m,n} = e^{\frac{i\phi_{m,n}}{2}} \mathbb{I} \end{cases}$$

$$\begin{cases} \mathcal{U}_{m,n} = \mathrm{Had}_a \sigma^X_a \, \mathrm{R}^Z_a(\phi_{m,n}) \mathrm{C}^X_{a,m} \mathrm{C}^X_{a,n} \left(\prod_{l=m}^{n-1} \mathrm{C}^{\tilde{X}}_{a,l} \right) \sigma^X_a \\ D_{m,n} = |C_{m,n}| \left(\frac{\mathbb{I}_m - \sigma^z_m}{2} \right) \left(\frac{\mathbb{I}_n - \sigma^z_n}{2} \right) \left(\prod_{l=m+1}^{n-1} \sigma^z_l \right) \sigma^z_a \end{cases}$$

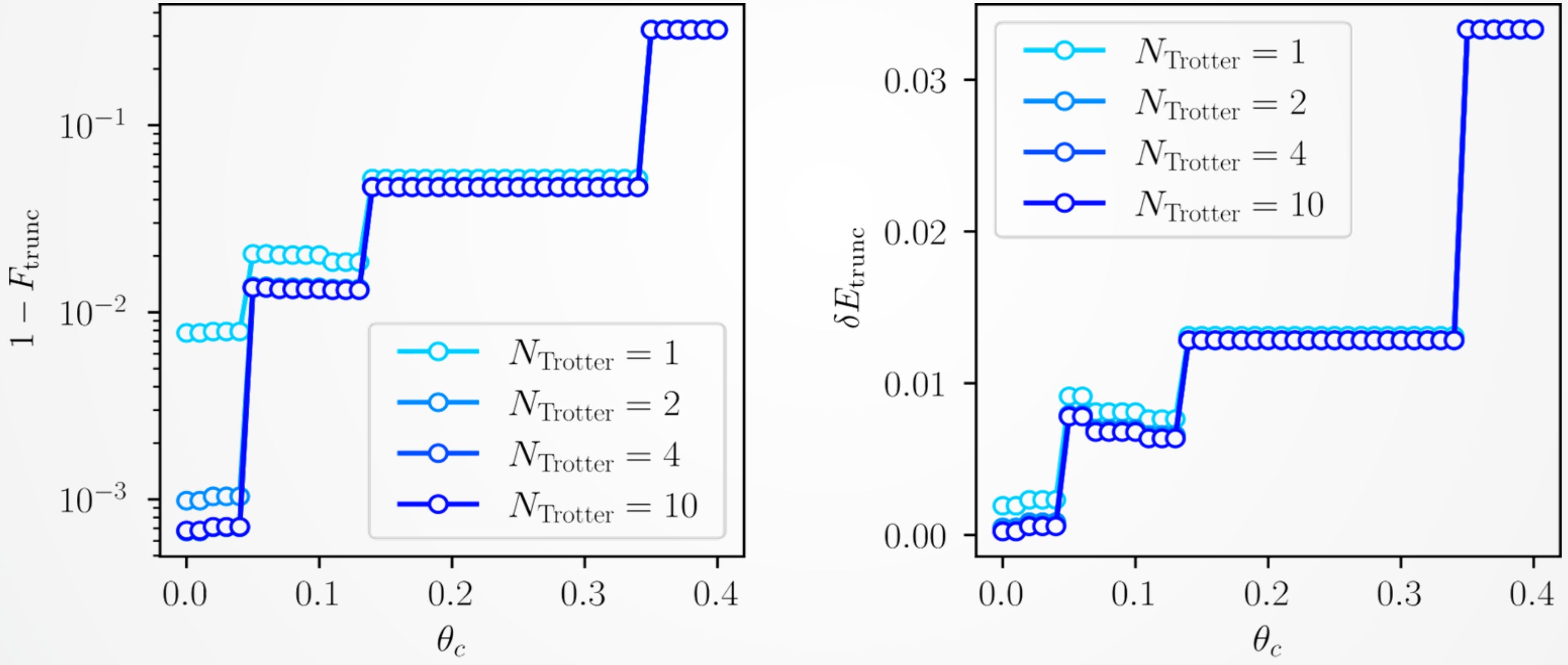
Angle truncation and Trotter steps

CNOTs count	$\mathcal{U}$	$\mathcal{D}$	Total
Ground state	$-$	$-$	$6N$
Wave packet (full)	$\frac{1}{4}N^3 + \frac{5}{2}N^2$	$\frac{1}{2}N^3 + 5N^2 + 2N$	$(N^3 + 10N^2 + 2N) \times 2N_{\text{trotter}}$
Wave packet (1-length)	$6N$	$14N$	$26N \times 2N_{\text{trotter}}$

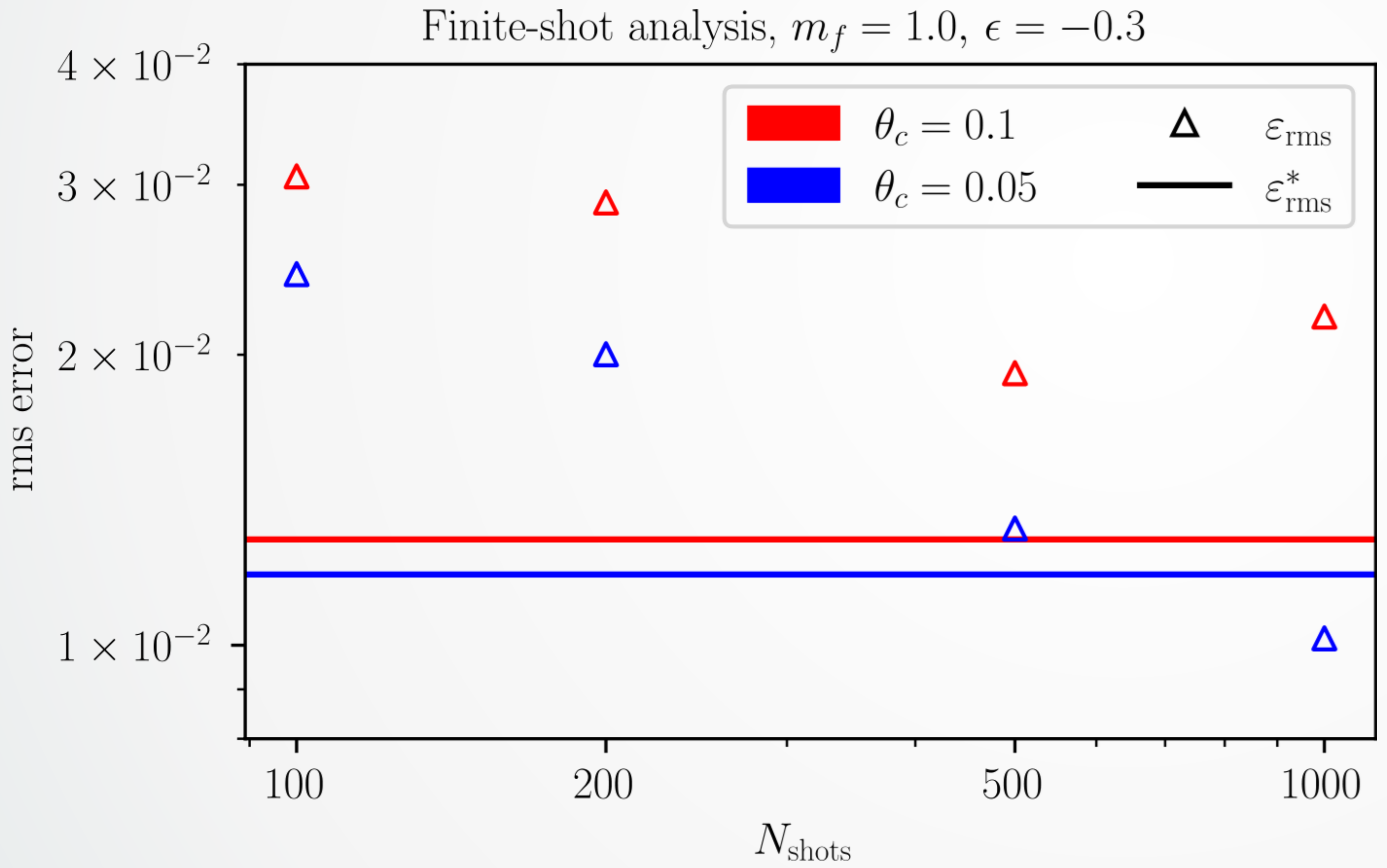


- **Trotterization**
  - 2nd order Trotterization
  - Fast saturation with N_{trotter}
- **Truncation:**
  - Only implement mesonic operators with $|C_{m,n}| > \theta_c$. $\mathcal{O}(N)$ gates for 1-length mesons
- **Parameters in actual implementation:**
  - $\theta_c = 0.1, N_{\text{trotter}} = 1$

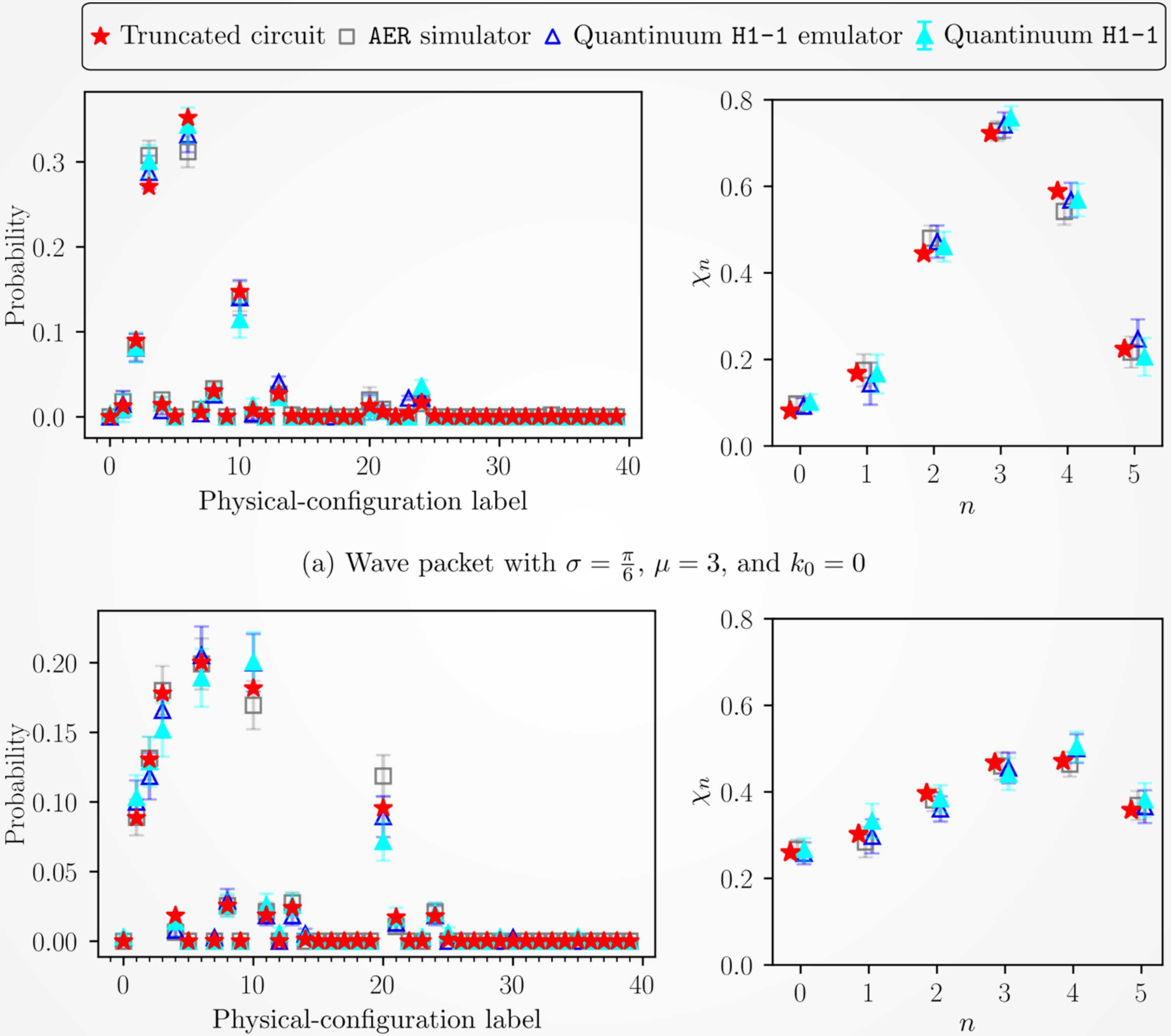
Trotter steps



Finite shot analysis



$$\varepsilon_{rms} = \sqrt{\sum_{i}^{N_H} \frac{\left(P^i_{shots} - P^i_{trunc}\right)^2}{N_H}}$$



(a) Wave packet with $\sigma = \frac{\pi}{6}$, $\mu = 3$, and $k_0 = 0$

(b) Wave packet with $\sigma = \frac{\pi}{10}$, $\mu = 3$, and $k_0 = 0$

Circuit: gate count

Option	N_{qubits}	$\mathcal{U},\mathcal{U}^\dagger$		D		$Total$
		One op.	Total	One op.	Total	
Z_2, GS	$2N_{site}$	2	$4N_{site}$	2	$2N_{site}$	$6N_{site}$
Z_2, WP	$2N_{site} + 1$	$0, L = 0$ $2 + L$, else	$\frac{1}{4}N_{site}^3 + \frac{5}{2}N_{site}^2$	$2, L = 0$ $6 + 2L$, else	$\frac{1}{2}N_{site}^3 + 5N_{site}^2 + 2N_{site}$	$2N_{trotter} \cdot \left(N_{site}^3 + 10N_{site}^2 + 2N_{site}\right)$
Z_2, WP, $L \leq 1$ mesons	$2N_{site} + 1$	$0, L = 0$ 3, else	$6N_{site}$	$2, L = 0$ 6, else	$14N_{site}$	$N_{trotter} \cdot 26N_{site}$
$U(1)$ WP, $\Lambda = 1$	$3N_{site} + 1$	$0, L = 0$ $2 + 4L$, else	$\frac{1}{2}N_{site}^3 + 2N_{site}^2$	$2, L = 0$ $6 + 2L$, else	$\frac{1}{2}N_{site}^3 + 5N_{site}^2 + 2N_{site}$	$2N_{trotter} \cdot \left(\frac{5}{2}N_{site}^3 + 13N_{site}^2 + 2N_{site}\right)$
$U(1)$ WP, $\Lambda = 1$, $L \leq 1$ mesons	$3N_{site} + 1$	$6, L = 0$ 6, else	$12N_{site}$	$2, L = 0$ 6, else	$14N_{site}$	$N_{trotter} \cdot 38N_{site}$

Physical-configuration label	$\|0\rangle_f$	$\|0\rangle_b$	$\|1\rangle_f$	$\|1\rangle_b$	$\|2\rangle_f$	$\|2\rangle_b$	$\|3\rangle_f$	$\|3\rangle_b$	$\|4\rangle_f$	$\|4\rangle_b$	$\|5\rangle_f$	$\|5\rangle_b$
0	0	0	1	0	0	0	1	0	0	0	1	0
1	1	1	0	0	0	0	1	0	0	0	1	0
2	0	0	0	1	1	0	1	0	0	0	1	0
3	0	0	1	0	1	1	0	0	0	0	1	0
4	1	1	0	0	1	1	0	0	0	0	1	0
5	1	1	1	1	0	1	0	0	0	0	1	0
6	0	0	1	0	0	0	0	1	1	0	1	0
7	1	1	0	0	0	0	0	1	1	0	1	0
8	0	0	0	1	1	0	0	1	1	0	1	0
9	0	0	0	1	0	1	1	1	1	0	1	0
10	0	0	1	0	0	0	1	0	1	1	0	0
11	1	1	0	0	0	0	1	0	1	1	0	0
12	0	0	0	1	1	0	1	0	1	1	0	0
13	0	0	1	0	1	1	0	0	1	1	0	0
14	1	1	0	0	1	1	0	0	1	1	0	0
15	1	1	1	1	0	1	0	0	1	1	0	0
16	1	1	1	1	1	0	0	1	0	1	0	0
17	0	0	1	0	1	1	1	1	0	1	0	0
18	1	1	0	0	1	1	1	1	0	1	0	0
19	1	1	1	1	0	1	1	1	0	1	0	0
20	1	0	1	0	0	0	1	0	0	0	0	1
21	1	0	0	1	1	0	1	0	0	0	0	1
22	0	1	1	1	1	0	1	0	0	0	0	1
23	1	0	1	0	1	1	0	0	0	0	0	1
24	1	0	1	0	0	0	0	1	1	0	0	1
25	1	0	0	1	1	0	0	1	1	0	0	1
26	0	1	1	1	1	0	0	1	1	0	0	1
27	0	1	0	0	1	1	1	1	1	0	0	1
28	1	0	0	1	0	1	1	1	1	0	0	1
29	0	1	1	1	0	1	1	1	1	0	0	1
30	0	1	0	0	0	0	1	0	1	1	1	1
31	0	1	0	0	1	1	0	0	1	1	1	1
32	1	0	0	1	0	1	0	0	1	1	1	1
33	0	1	1	1	0	1	0	0	1	1	1	1
34	1	0	1	0	0	0	0	1	0	1	1	1
35	1	0	0	1	1	0	0	1	0	1	1	1
36	0	1	1	1	1	0	0	1	0	1	1	1
37	0	1	0	0	1	1	1	1	0	1	1	1
38	1	0	0	1	0	1	1	1	0	1	1	1
39	0	1	1	1	0	1	1	1	0	1	1	1

Physical-configuration label	$\|0\rangle_f$	$\|0\rangle_b$	$\|1\rangle_f$	$\|1\rangle_b$	$\|2\rangle_f$	$\|2\rangle_b$	$\|3\rangle_f$	$\|3\rangle_b$	$\|4\rangle_f$	$\|4\rangle_b$	$\|5\rangle_f$	$\|5\rangle_b$
0	1	0	1	0	1	−1	0	0	0	0	0	1
1	1	−1	1	−1	0	−1	1	−1	0	−1	0	0
2	1	0	1	0	0	0	1	0	0	0	0	1
3	1	−1	0	0	1	−1	1	−1	0	−1	0	0
4	1	0	0	1	1	0	1	0	0	0	0	1
5	0	0	1	0	1	−1	1	−1	0	−1	0	0
6	0	1	1	1	1	0	1	0	0	0	0	1
7	1	−1	1	−1	0	−1	0	0	1	−1	0	0
8	1	0	1	0	0	0	0	1	1	0	0	1
9	1	−1	0	0	1	−1	0	0	1	−1	0	0
10	1	0	0	1	1	0	0	1	1	0	0	1
11	0	0	1	0	1	−1	0	0	1	−1	0	0
12	0	1	1	1	1	0	0	1	1	0	0	1
13	1	−1	0	0	0	0	1	0	1	−1	0	0
14	1	0	0	1	0	1	1	1	1	0	0	1
15	0	0	1	0	0	0	1	0	1	−1	0	0
16	0	1	1	1	0	1	1	1	1	0	0	1
17	0	0	0	1	1	0	1	0	1	−1	0	0
18	1	−1	1	−1	0	−1	0	0	0	0	1	0
19	1	0	1	0	0	0	0	1	0	1	1	1
20	1	−1	0	0	1	−1	0	0	0	0	1	0
21	1	0	0	1	1	0	0	1	0	1	1	1
22	0	0	1	0	1	−1	0	0	0	0	1	0
23	0	1	1	1	1	0	0	1	0	1	1	1
24	1	−1	0	0	0	0	1	0	0	0	1	0
25	1	0	0	1	0	1	1	1	0	1	1	1
26	0	−1	1	−1	0	−1	1	−1	0	−1	1	−1
27	0	0	1	0	0	0	1	0	0	0	1	0
28	0	1	1	1	0	1	1	1	0	1	1	1
29	0	−1	0	0	1	−1	1	−1	0	−1	1	−1
30	0	0	0	1	1	0	1	0	0	0	1	0
31	1	−1	0	0	0	0	0	1	1	0	1	0
32	0	−1	1	−1	0	−1	0	0	1	−1	1	−1
33	0	0	1	0	0	0	0	1	1	0	1	0
34	0	−1	0	0	1	−1	0	0	1	−1	1	−1
35	0	0	0	1	1	0	0	1	1	0	1	0
36	0	−1	0	0	0	0	1	0	1	−1	1	−1
37	0	0	0	1	0	1	1	1	1	0	1	0