Towards simulate Fermionic Scattering on a QC

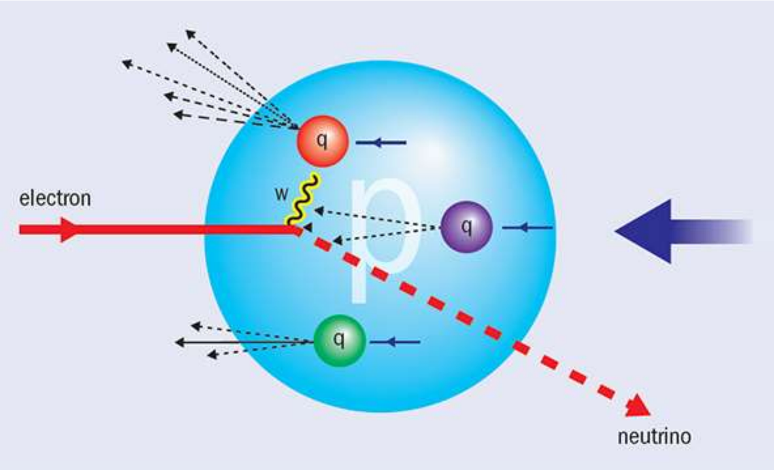
Yahui Chai, Arianna Crippa, Karl Jansen, Stefan Kuehn,
Vincent R. Pascuzzi, Francesco Tacchino, and Ivano Tavernelli

DESY. QUANTUM
Center for
Quantum Technology
and Applications

Motivation

- Real time dynamics in classical simulation
  - Conventional Monte Carlo: sign problem
  - Tensor Network : increasing entanglement with time-- increasing computation resource
- Quantum computers promise to efficiently simulate real-time dynamics
- Necessary steps for simulating scattering

① Preparing the ground state
② <u>Creating wave packets on top, which represent particles</u>
③ Evolving the resulting state in time
④ Measuring relevant observables



Outline

- Theoretical set up
  - The Thirring model
  - Preparation for wave packet using quantum circuit

- Simulation results
  - Classical simulation for noninteracting and interacting case
  - Quantum simulation for noninteracting case

The Thirring model

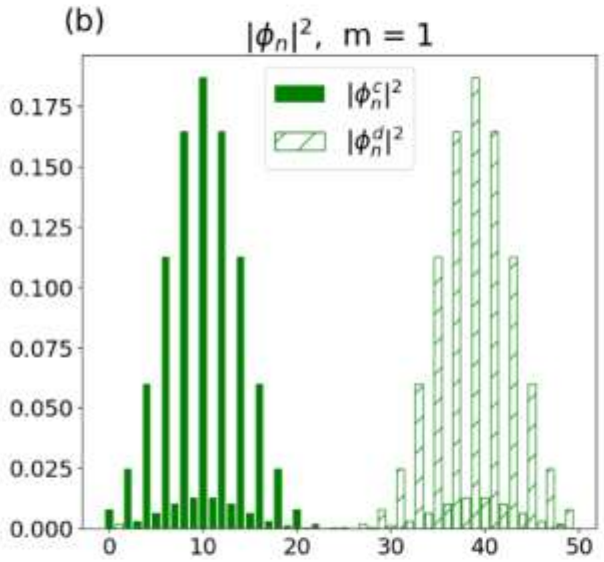
$$H = \sum_{n=0}^{N-1} \frac{i}{2a} \underbrace{\left(\xi_{n+1}^{\dagger}\xi_n - \xi_n^{\dagger}\xi_{n+1}\right)}_{\text{Kinetic term}} + m \sum_{n=0}^{N-1} \underbrace{(-1)^n \xi_n^{\dagger}\xi_n}_{\text{Mass term}} + \frac{g}{a} \sum_{n=0}^{N-1} \underbrace{\xi_n^{\dagger}\xi_n\xi_{n+1}^{\dagger}\xi_{n+1}}_{\text{Four-body interaction}}$$

- Exactly solvable fermionic model in 1+1 dimension, Kogut-Susskind formula
- $\xi_n^{\dagger}, \xi_n$: fermionic creation or annihilation operators
- a: lattice spacing, a = 1
- Periodic boundary condition: $\xi_N = \xi_0$

Scattering process

✓Vacuum state $|\Omega\rangle$: ground state of Hamiltonian H

- Initial state $|\psi(0)\rangle$: wave packets of particles



✓Time evolution : $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$

Define wave packets in momentum space

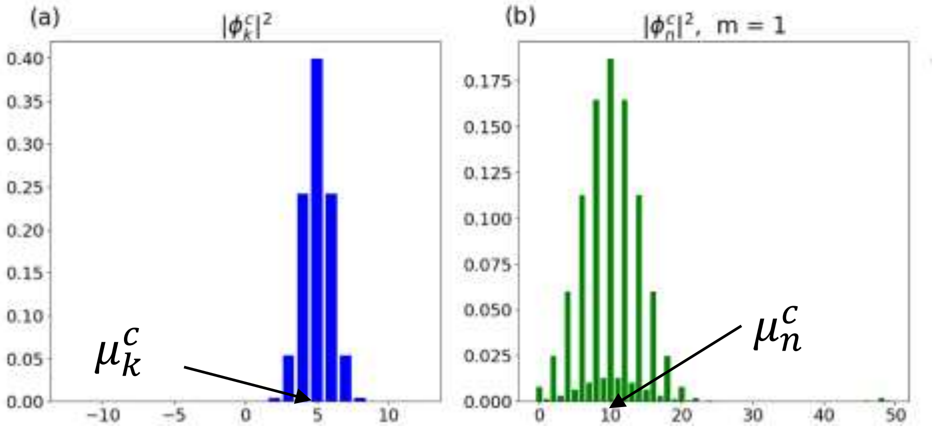
- Creation operators for fermion and antifermion wave packets

$$C^\dagger(\phi^c) = \sum_k \phi_k^c c_k^\dagger \qquad c_k^\dagger = \frac{1}{\sqrt{N}}\sqrt{\frac{m+w_k}{w_k}}\sum_n e^{ikn}\left(\Pi_{n0} + v_k\Pi_{n1}\right)\xi_n^\dagger$$

$$D^\dagger(\phi^d) = \sum_k \phi_k^d d_k^\dagger \qquad d_k^\dagger = \frac{1}{\sqrt{N}}\sqrt{\frac{m+w_k}{w_k}}\sum_n e^{ikn}\left(\Pi_{n1} + v_k\Pi_{n0}\right)\xi_n$$

- Amplitude of Gaussian Wave packet in momentum space

$$\phi_k^{c(d)} = \frac{1}{\mathcal{N}_k^{c(d)}} e^{-ik\underset{\underset{\text{Position}}{\downarrow}}{\mu_n^{c(d)}}} e^{-(k-\underset{\underset{\text{Momentum}}{\downarrow}}{\mu_k^{c(d)}})^2/4\underset{\underset{\text{Width}}{\downarrow}}{\sigma_k^2}}$$



Define wave packets in position space

- Momentum space

$C^\dagger(\phi^c)$ $$\sum_k \phi_k^c c_k^\dagger$$

$D^\dagger(\phi^d)$ $$\sum_k \phi_k^d d_k^\dagger$$

$$\phi_k^{c(d)} = \frac{1}{\mathcal{N}_k^{c(d)}} e^{-ik\mu_n^{c(d)}} e^{-(k-\mu_k^{c(d)})^2/4\sigma_k^2}$$

Fourier transformation:

$c_k^\dagger \to \xi_n^\dagger$

$d_k^\dagger \to \xi_n$

- Position space

$$\sum_n \phi_n^c \xi_n^\dagger$$

$$\sum_n \phi_n^d \xi_n$$

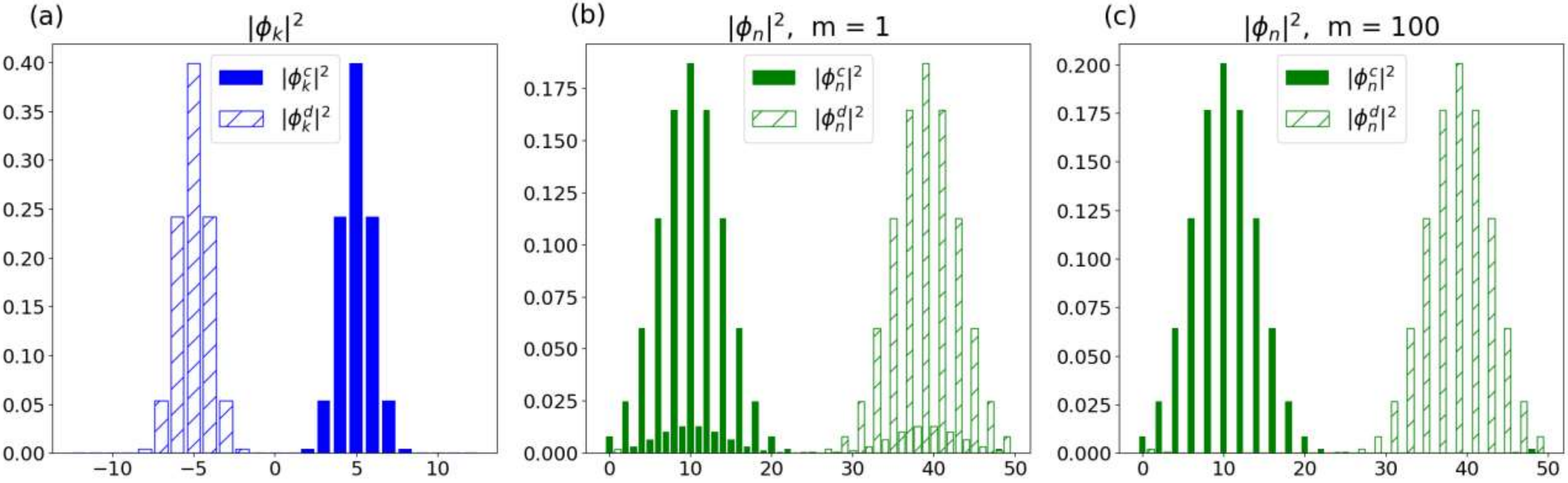
$|v_k| \leq 1$

$$\phi_n^c = \frac{1}{\sqrt{N}} \sum_k \phi_k^c \sqrt{\frac{m+w_k}{w_k}} e^{ikn} \left(\Pi_{n0} + v_k \Pi_{n1}\right)$$

$$\phi_n^d = \frac{1}{\sqrt{N}} \sum_k \phi_k^d \sqrt{\frac{m+w_k}{w_k}} e^{ikn} \left(\Pi_{n1} + v_k \Pi_{n0}\right)$$

Preparation of wave packets

$m\uparrow, |v_k|\downarrow$



- Fermions mainly locate at even site
- Antifermions mainly locate at odd site

Summary for operators

- Initial state: $|\psi(0)\rangle = D^\dagger(\phi^d)\, C^\dagger(\phi^c)|\Omega\rangle$

$$C^\dagger(\phi^c) = \sum_n \phi_n^c \xi_n^\dagger, \qquad D^\dagger(\phi^d) = \sum_n \phi_n^d \xi_n$$

$$\phi_n^c(\mu_k^c, \mu_n^c, \sigma_k^c), \quad \phi_n^d(\mu_k^d, \mu_n^d, \sigma_k^d)$$

- **How to implement the linear combination of operators in a quantum computing?**

Operator for linear transformation

- Suppose ϕ_n^c is the first column of an unitary matrix

$$C^\dagger(\phi_n^c) = \sum_{n=0}^{N-1} \xi_n^\dagger u_{n0}$$

Four sites example

$$\begin{pmatrix} C^\dagger(\phi^c) & * & * & * \end{pmatrix} = \begin{pmatrix} \xi_0^\dagger & \xi_1^\dagger & \xi_2^\dagger & \xi_3^\dagger \end{pmatrix} \cdot \begin{pmatrix} \phi_0^c & * & * & * \\ \phi_1^c & * & * & * \\ \phi_2^c & * & * & * \\ \phi_3^c & * & * & * \end{pmatrix}$$

- Unitary operators for linear transformation

$$V(u)\xi_0^\dagger V^\dagger(u) = \sum_n \xi_n^\dagger u_{n0}$$

$$V(u) = \exp\left(\sum_{nl} [\log u]_{nl} \; \xi_n^\dagger \xi_l\right)$$

Decompose $V(u)$

- The unitary transformation is a homomorphism under matrix multiplication

$$V(u \times u') = V(u) \times V(u')$$

- If we can decompose u in a product of matrices acting only on a few sites nontrivially, V(u) can be represented as series of local gates
  - The matrix u can be decomposed using Givens rotation

$$u = p(\vec{\beta})^\dagger \cdot r_{N-1}(\theta_{N-1})^\dagger \cdots r_1(\theta_1)^\dagger$$

  - Translate the fermions to spins using a Jordan-Wigner transformation

Z. Jiang et al., Phys. Rev. Appl. 9, 044036 (2018)

Decompose $V(u)$

$$V(u \times u') = V(u) \times V(u')$$

$$u = p(\vec{\beta})^\dagger \cdot r_{N-1}(\theta_{N-1})^\dagger \cdots r_1(\theta_1)^\dagger$$

$$V(\phi^c) := \quad V(u) = V^\dagger(p) \cdot V^\dagger(r_{N-1}) \cdots V^\dagger(r_1)$$

$$V^\dagger(p) = \exp\left(-i \sum_n \beta_n \; \xi_n^\dagger \xi_n\right)$$

$$V^\dagger(r_n) = \exp\left(\theta_n [\xi_{n-1}^\dagger \xi_n - \xi_n^\dagger \xi_{n-1}]\right)$$

Jordan-Wigner transformation

$$V^\dagger(p) = \exp\left(i \sum_n \beta_n \; \sigma_n^z\right)$$

$$V^\dagger(r_n) = \exp\left(i \frac{\theta_n}{2} \left[\sigma_{n-1}^x \sigma_n^y - \sigma_{n-1}^y \sigma_n^x\right]\right)$$

Summary of wave packet preparation

- Initial state: $|\psi(0)\rangle = D^\dagger(\phi^d)\ C^\dagger(\phi^c)\,|\Omega\rangle$

$$C^\dagger(\phi^c) = \sum_n \phi_n^c \xi_n^\dagger, \qquad D^\dagger(\phi^d) = \sum_n \phi_n^d \xi_n$$

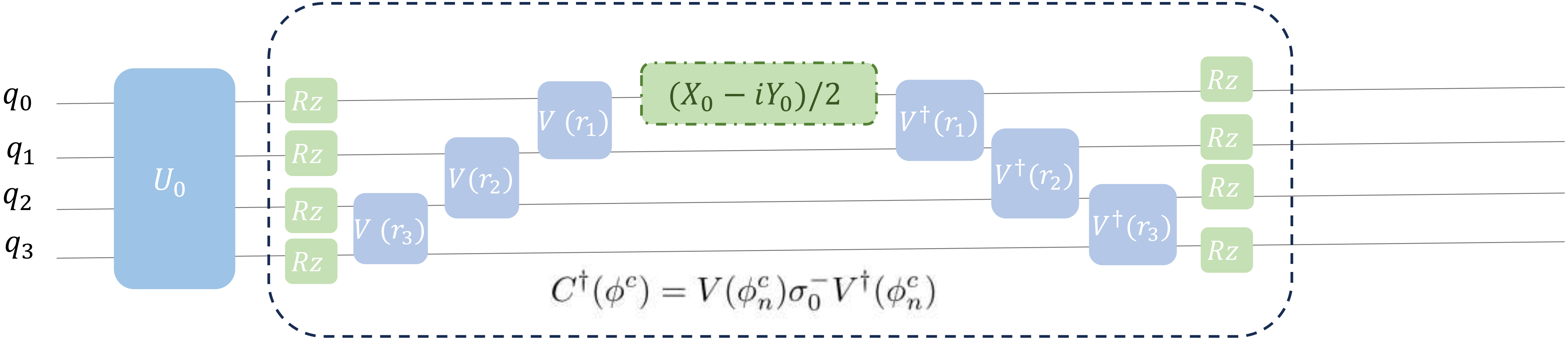
- Unitary operator $V\left(\phi^{c(d)}\right)$

$$C^\dagger(\phi^c) = V(\phi^c)\xi_0^\dagger V^\dagger(\phi^c), \qquad D^\dagger(\phi^d) = V(\phi^{d*})\xi_0^\dagger V^\dagger(\phi^{d*})$$

- Decompose $V\left(\phi^{c(d)}\right)$ using Givens rotation

Circuit for wave packet preparation

$$\begin{aligned}|\psi(0)\rangle &= D^\dagger(\phi_n^d)C^\dagger(\phi_n^c)\,|\Omega\rangle \\ &= V(\phi_n^{d*})\xi_0 V^\dagger(\phi_n^{d*})\boxed{V(\phi_n^c)\xi_0^\dagger V^\dagger(\phi_n^c)}U_0\,|0\rangle\end{aligned}$$



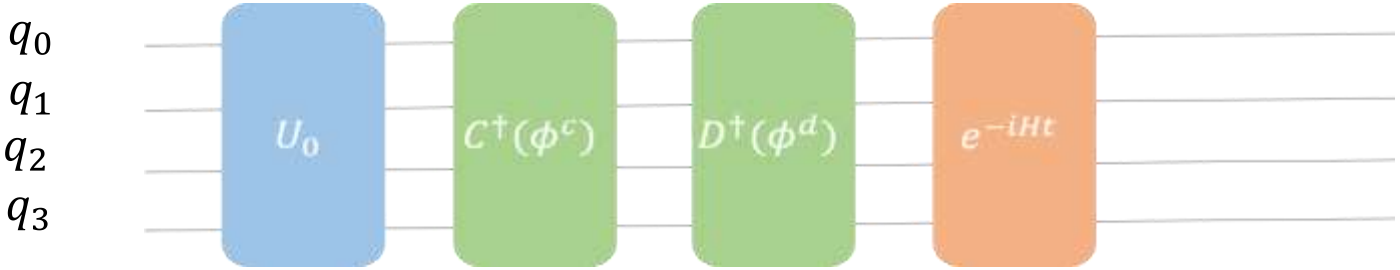
$$C^\dagger(\phi^c) = V(\phi_n^c)\sigma_0^- V^\dagger(\phi_n^c)$$

- Jordan-Wigner transformation

$$\xi_n^\dagger = \prod_{l<n} \sigma_l^z \sigma_n^-, \quad \xi_n = \prod_{l<n} \sigma_l^z \sigma_n^+$$

Circuit for scattering process

- Acting time evolution on initial state: $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$



- Since σ^+, σ^- is nonunitary, the circuit cannot be directly implemented
- We only care about expectation values of observables O which have the form

$$\langle O \rangle = \sum_{P_1,P_2,P_3,P_4} \gamma_{P_1P_2P_3P_4} \times$$

$$\langle \Omega | V(\phi^c) P_4 V^\dagger(\phi^c) V(\phi^{d*}) P_3 V^\dagger(\phi^{d*}) e^{iHt} \; O \; e^{-iHt} V(\phi^{d*}) P_2 V^\dagger(\phi^{d*}) V(\phi^c) P_1 V^\dagger(\phi^c) |\Omega\rangle$$

  - The P_k are just Pauli matrices, $P_k \in \{X, Y\}$, the coefficients are $\gamma_{P_1P_2P_3P_4} \in \{\pm 1, \pm i\}$
  - The individual terms can be measured with a variant of the Hadamard test

Observables

- Focus on the sector of $\sum_n \xi_n^\dagger \xi_n = N/2$
- Monitor the excess fermion density with respect to the ground state $|\Omega\rangle$ over time

$$\Delta\langle \xi_n^\dagger \xi_n \rangle_t = \langle \psi(t) | \xi_n^\dagger \xi_n | \psi(t) \rangle - \langle \Omega | \xi_n^\dagger \xi_n | \Omega \rangle$$

- Entropy difference with respect to the ground state

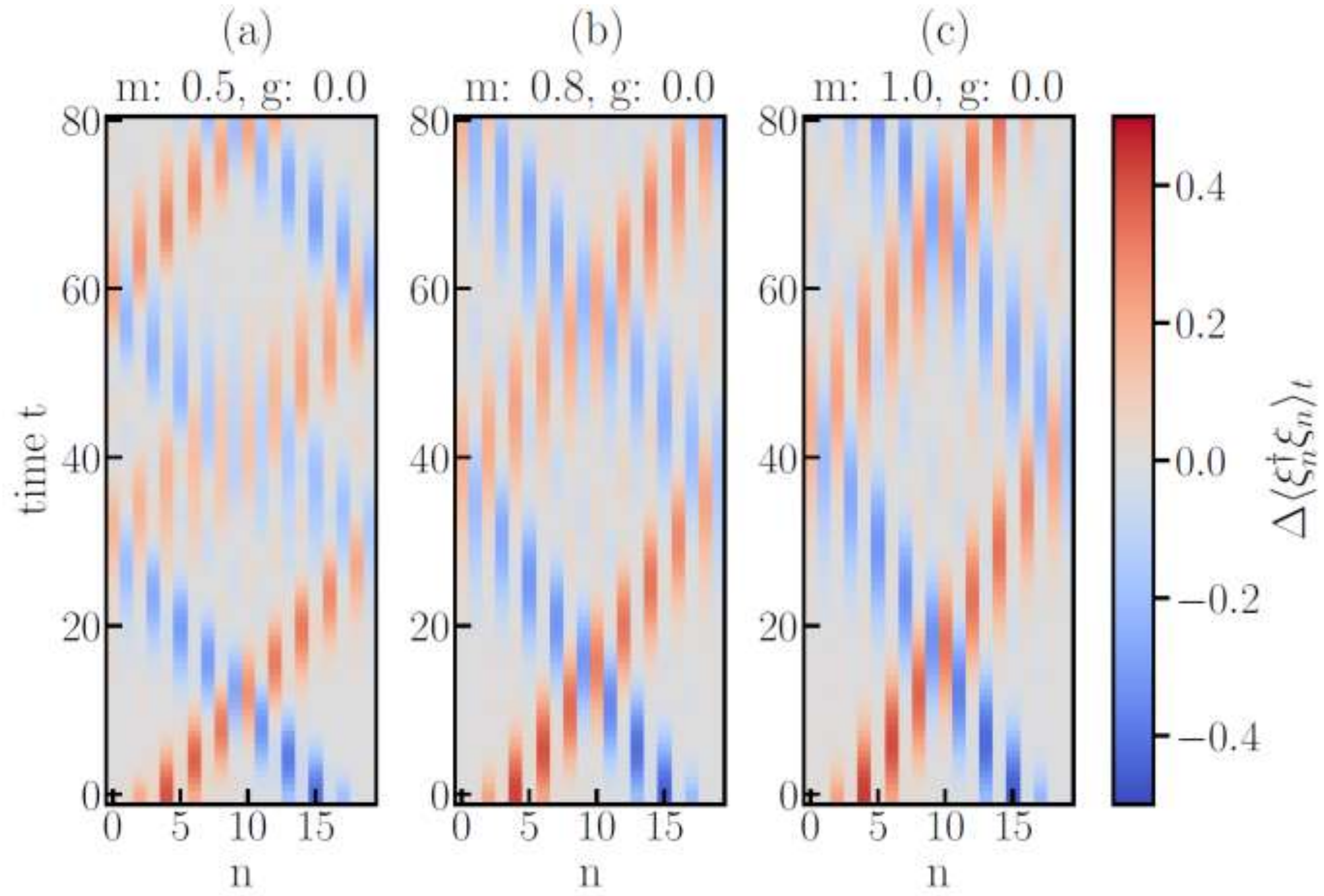
$$\Delta S_1(n,t) = S(n,t) - S_\Omega(n)$$

- Monitor the entropy production over time compared to two wave packets moving individually

$$\Delta S_2(n,t) = \Delta S_1(n,t) - (\Delta S_{1,C}(n,t) + \Delta S_{1,D}(n,t))$$

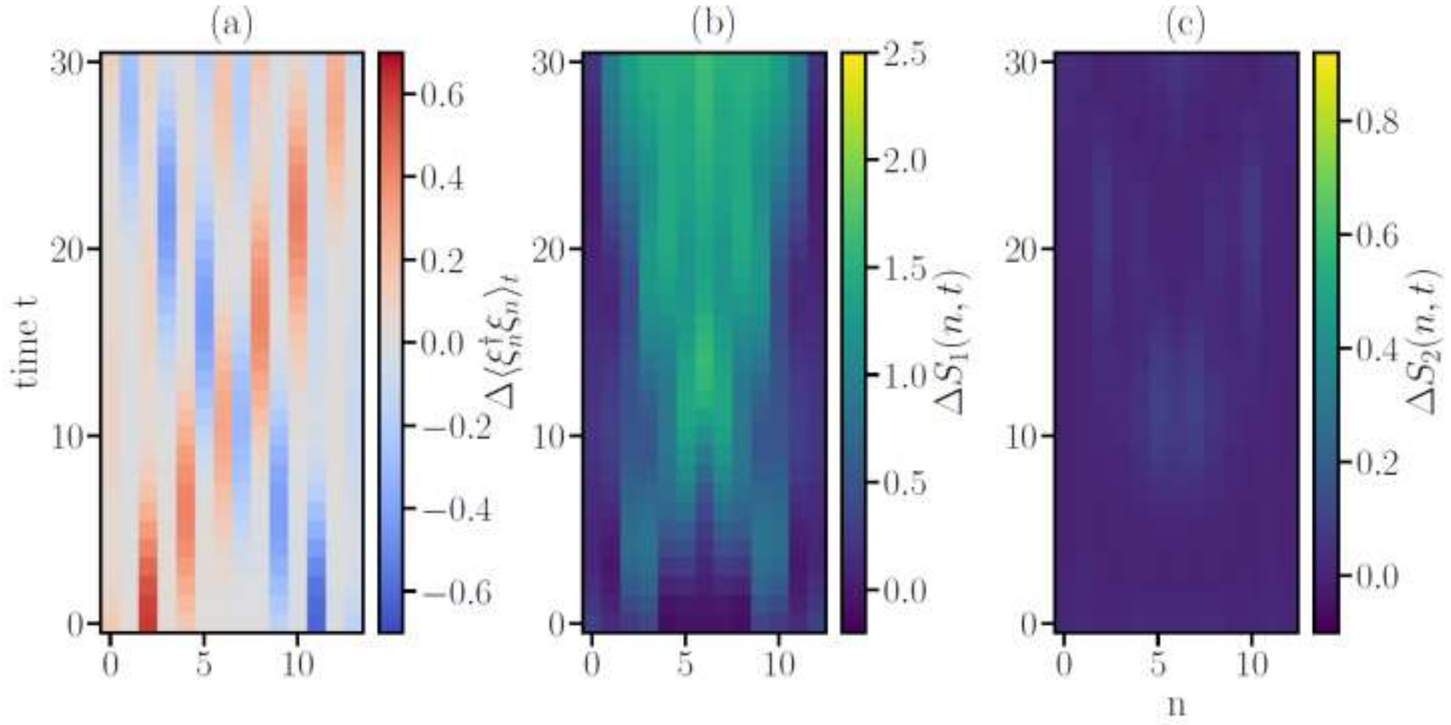
Classical simulation for the noninteracting case

Free fermion propagation: $g = 0$



- Wave packets show up as excess/lack in fermion density
- Particles move freely without interacting
- Larger mass leads to slower dynamics

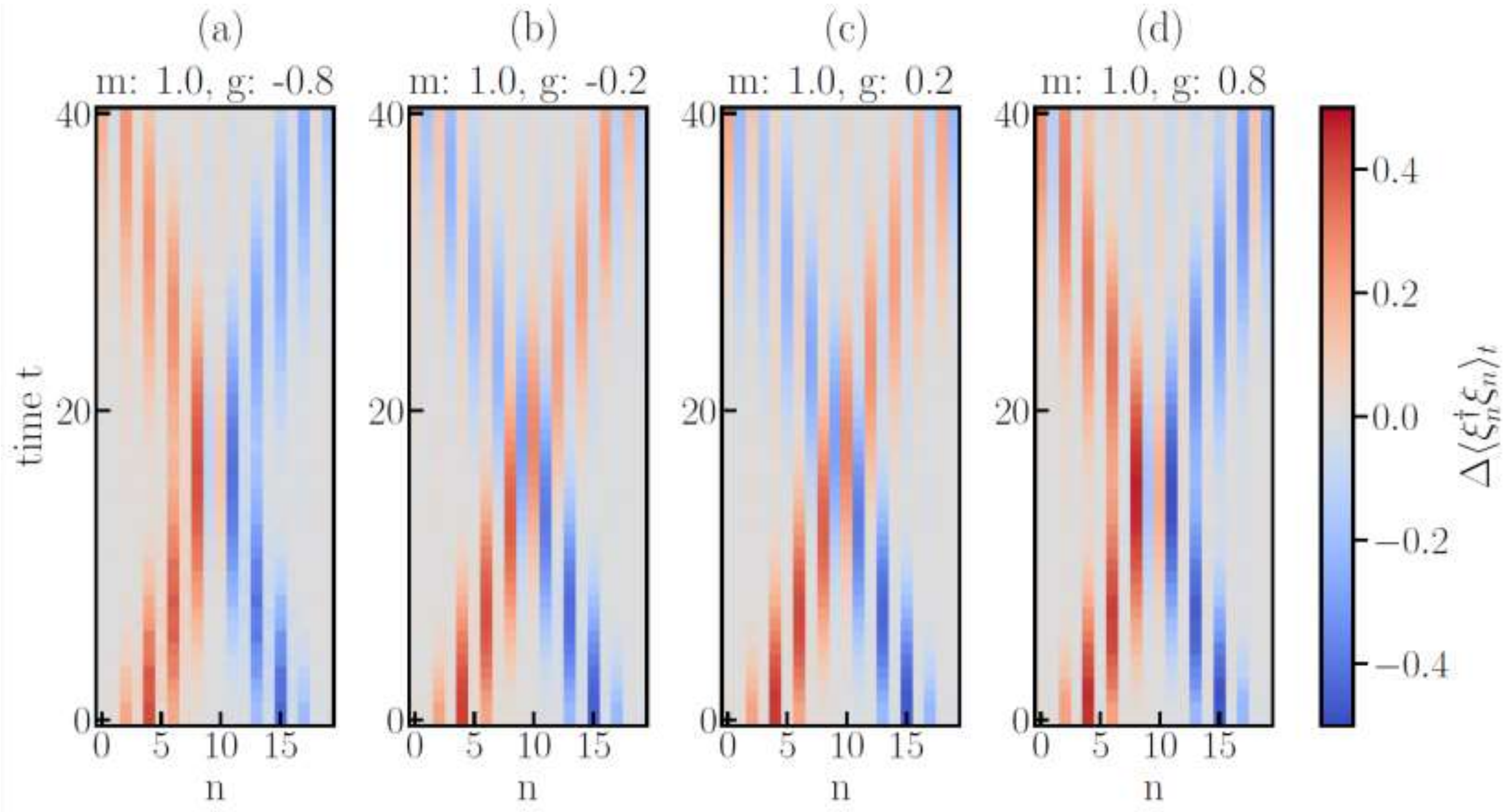
Free fermion propagation: $g = 0$



- $\Delta S_1(n,t)$ has a nonzero value, entropy change with respect to the ground state
- $\Delta S_2(n,t)$ is essentially zero
- No difference in entropy compared to two wave packets moving individually

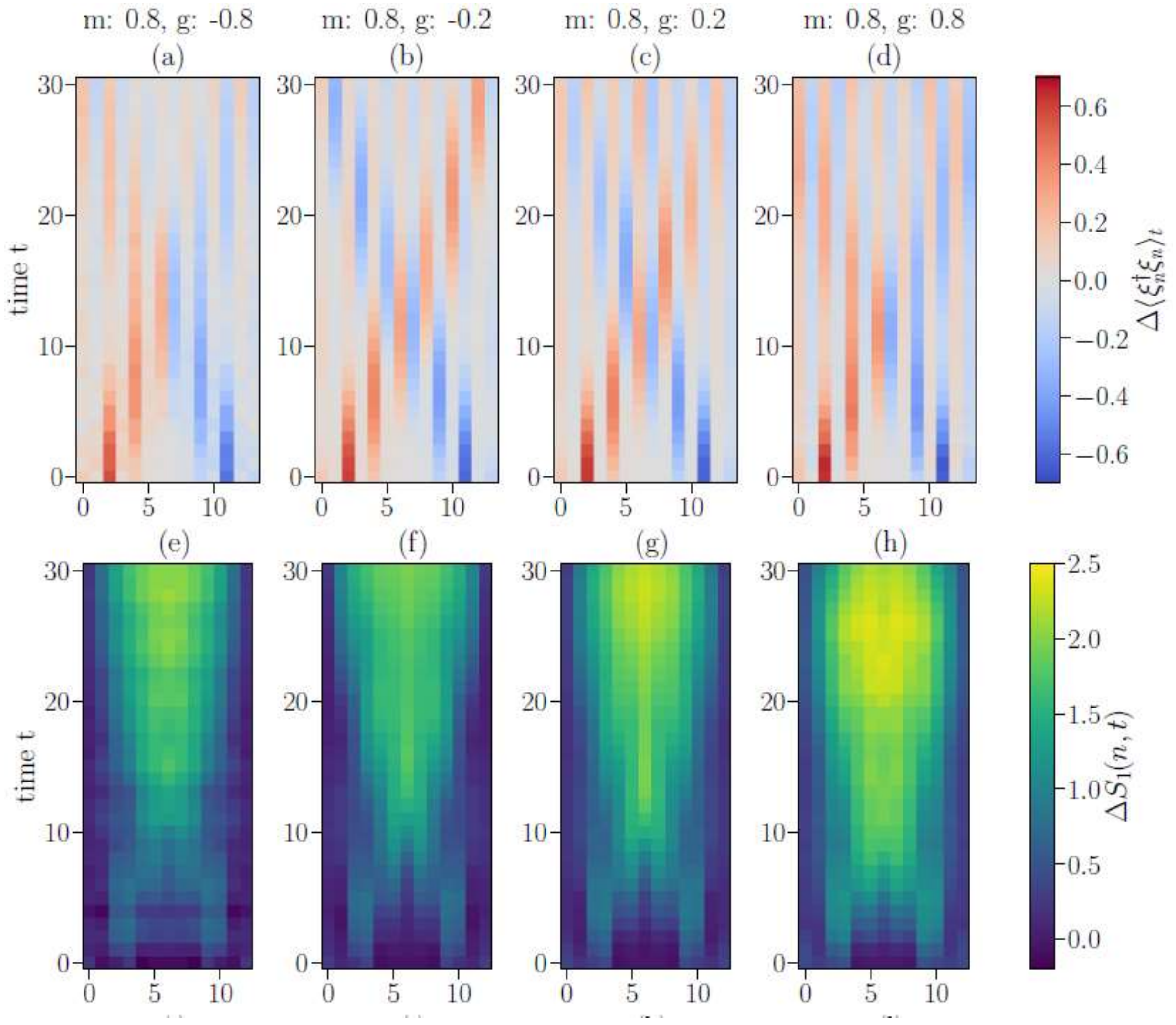
Classical simulation for the interacting case

Fermionic scattering: $\boldsymbol{g \neq 0}$



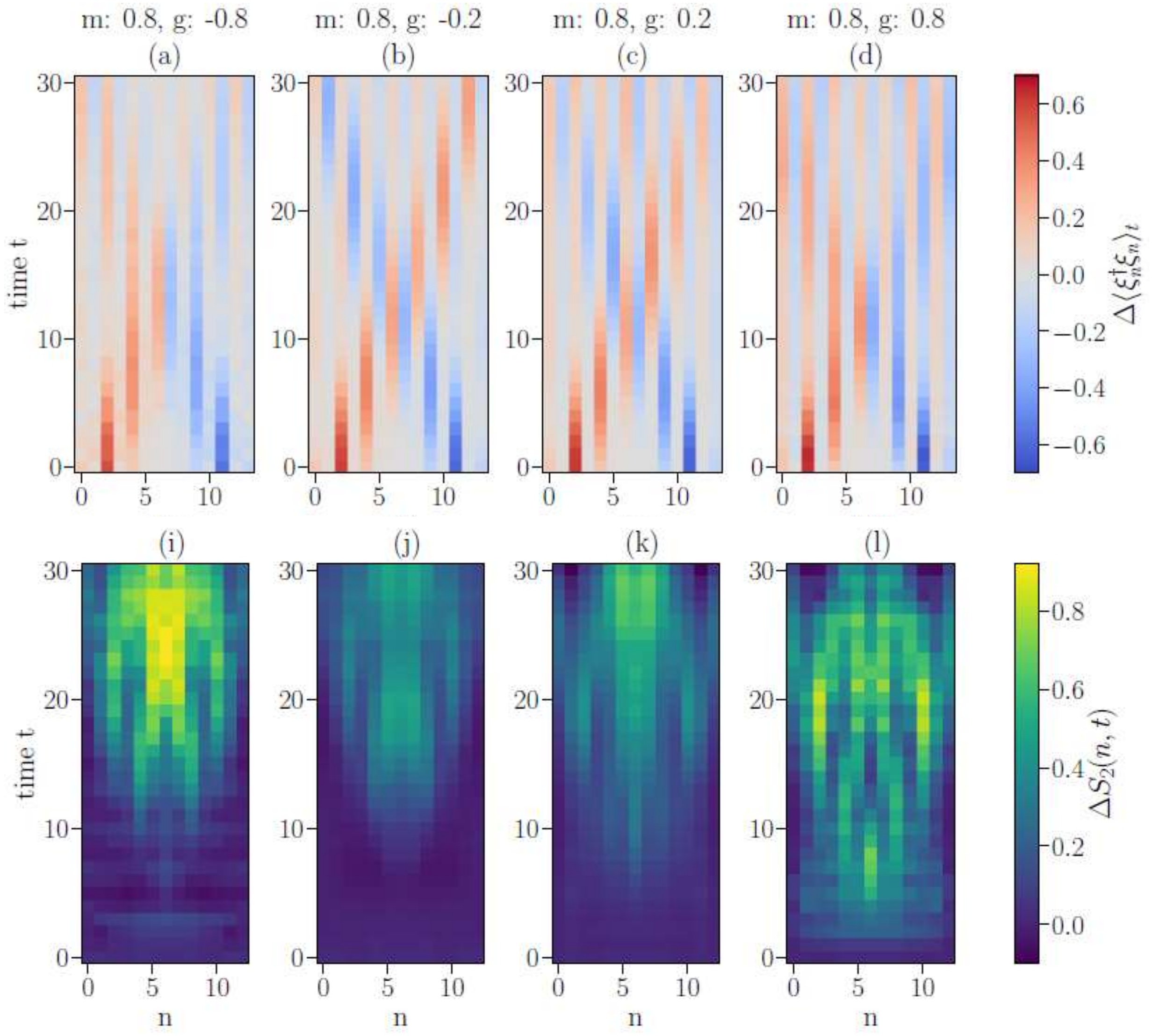
- Elastic scattering between the fermion and antifermion for large values of $|g|$

Fermionic scattering: $g \neq 0$



- We again observe excess entropy with respect to the vacuum

Fermionic scattering: $g \neq 0$



- We again observe excess entropy with respect to the vacuum

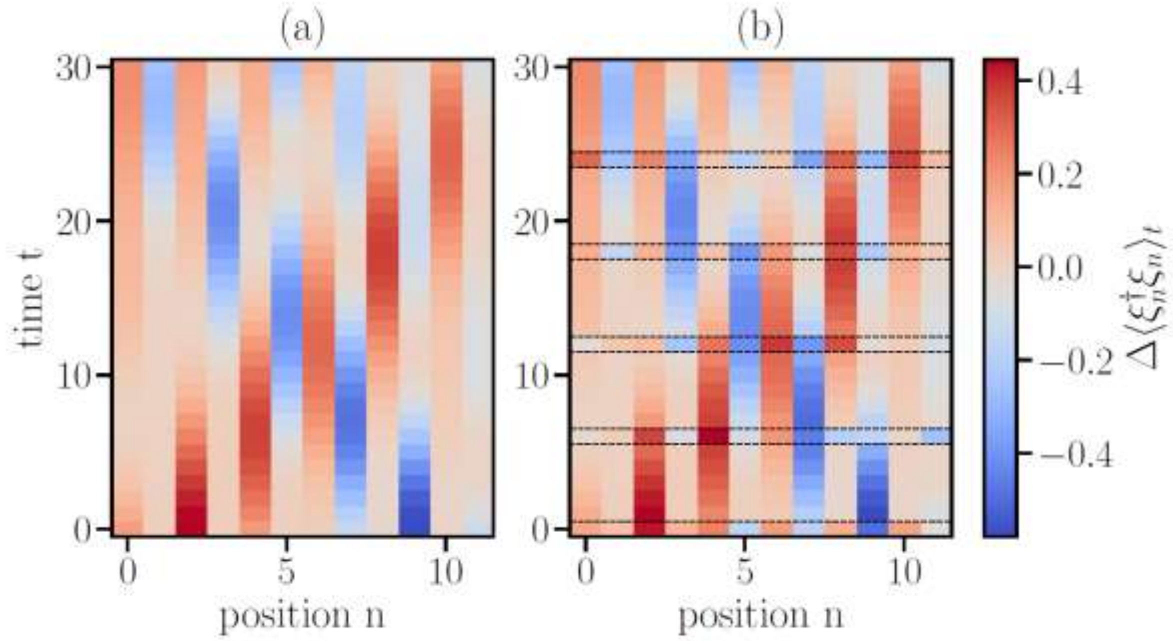
- This time $\Delta S_2(n,t)$after the Collision:
  - Effect of the interaction

- Entropy production is larger for larger values of $|g|$

Quantum simulation for the noninteracting case

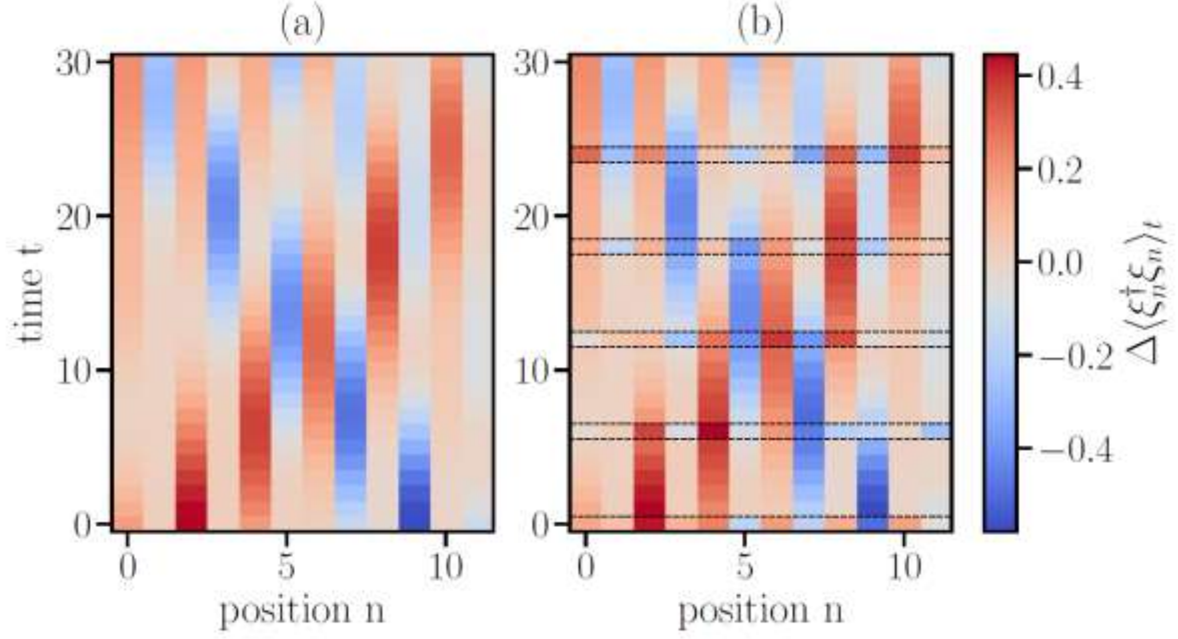
Quantum simulation: $g = 0$

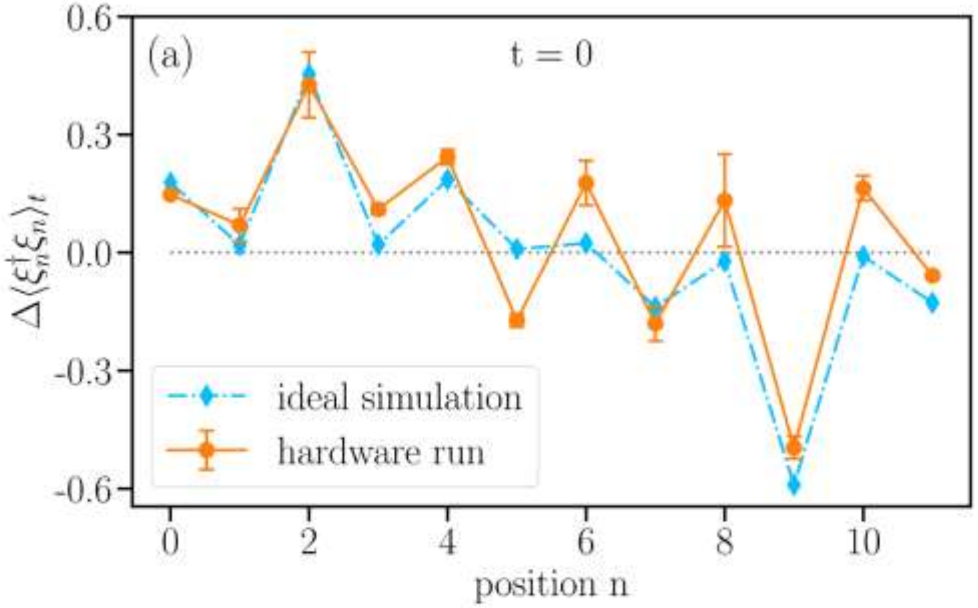
- Results from ibmq_peekskill after applying Pauli twirling, dynamical decoupling and zero noise extrapolation



Quantum simulation: $\boldsymbol{g = 0}$

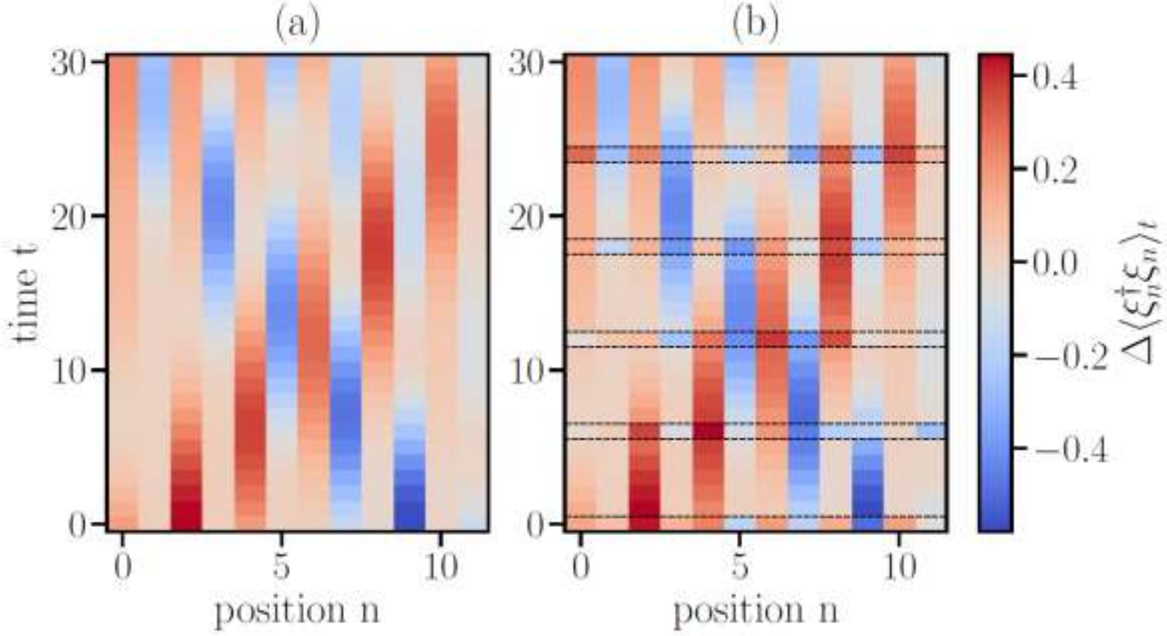
- Results from ibmq_peekskill after applying Pauli twirling, dynamical decoupling and zero noise extrapolation

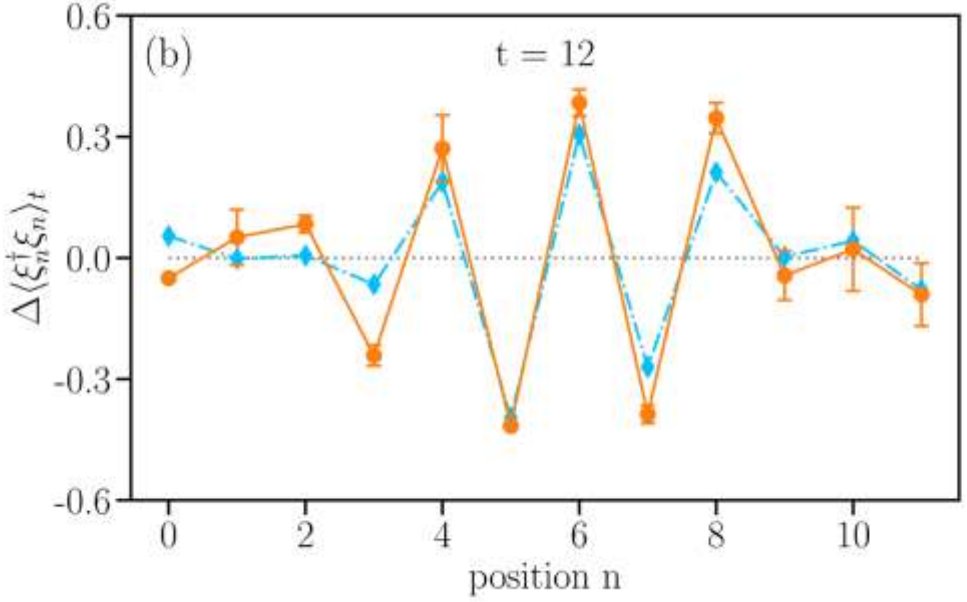




Quantum simulation: $g = 0$

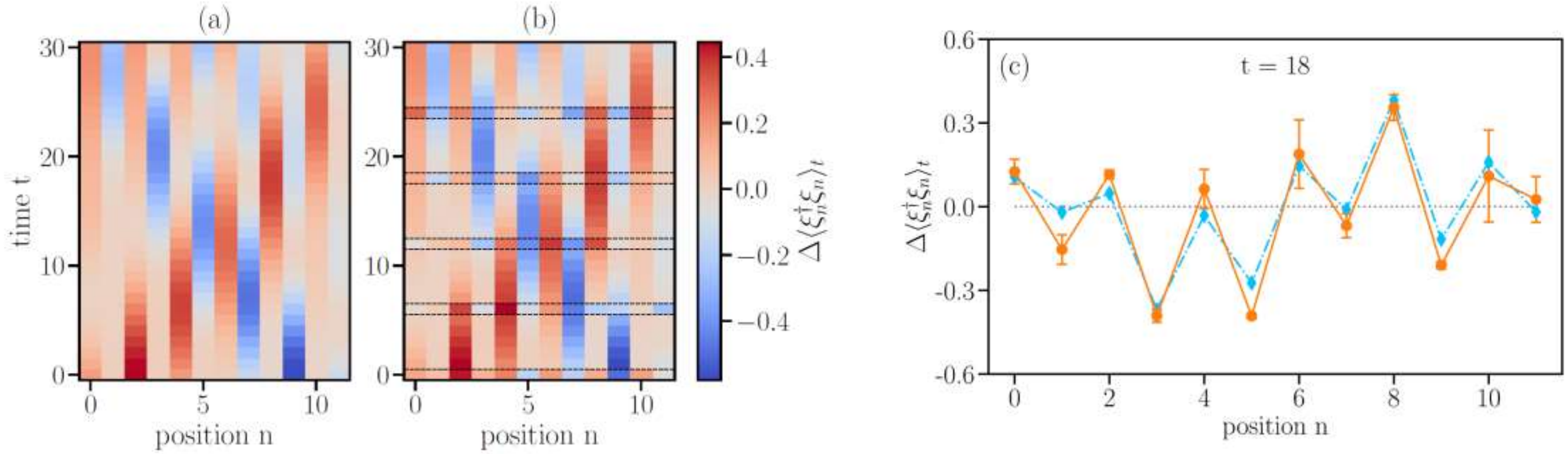
- Results from ibmq_peekskill after applying Pauli twirling, dynamical decoupling and zero noise extrapolation





Quantum simulation: $g = 0$

- Results from ibmq_peekskill after applying Pauli twirling, dynamical decoupling and zero noise extrapolation



Summary and outlooks

- Propose the framework to simulate fermionic scattering on a digital quantum computing approach.
  - Simulated the elastic scattering process in the Thirring model classicaly
  - Successful implementation for the noninteracting case on quantum hardware

- Outlook:
  - Study the interacting Thirring model on quantum hardware
  - Apply the method to other fermionic models
  - Extension to gauge models

Thank you!

Stefan Kühn
(CQTA)

Arianna Crippa
(CQTA)

Karl Jansen
(CQTA)

Vincent R.
Pascuzzi (IBM, NY)

Francesco
Tacchino (IBM
Zürich)

Ivano Tavernelli
(IBM Zürich)

arXiv:2312.02272

DESY. QUANTUM | Center for Quantum Technology and Applications