Quantum Simulation of the N-flavor Gross-Neveu (GN) Model

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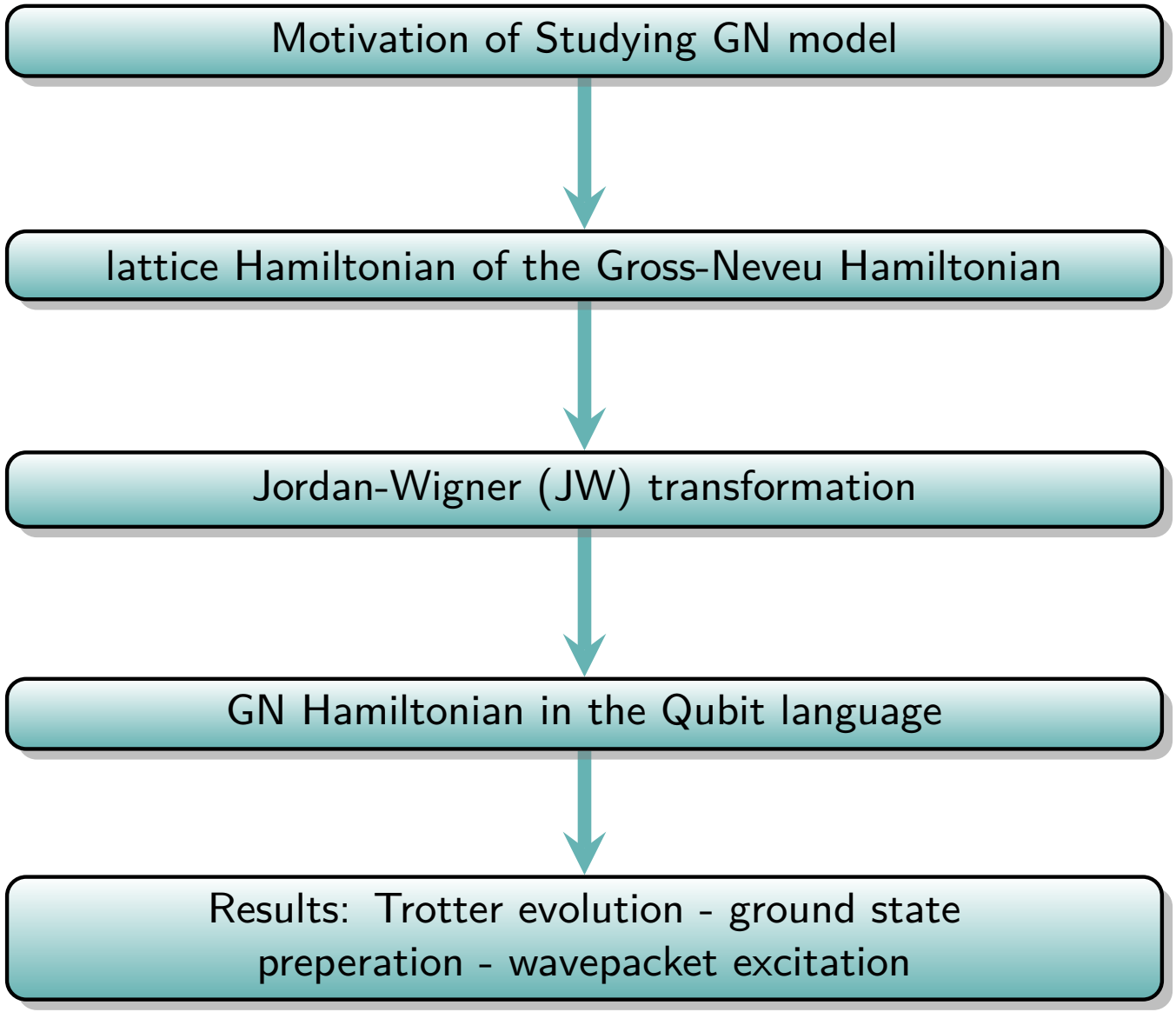
Outline


Motivation of Studying GN model
lattice Hamiltonian of the Gross-Neveu Hamiltonian
Jordan-Wigner (JW) transformation
GN Hamiltonian in the Qubit language
Results: Trotter evolution - ground state preperation - wavepacket excitation

Motivation

- GN model: shares many features of QCD

- asymptotically free theory
- dynamical mass generation without spontaneous symmetry breaking (Catterall *et.el.* 2018, 2021)
- Analytic computation possible in the $N \to \infty$ limit, like that of t'Hooft's large N_c limit for QCD

- N-component fermionic model with quartic interaction term - useful toy model to study with quantum computers
-Implication in the condensed matter physics

- Su-Schrieffer-Heeger (SSH) model of polyacetylen
- $N = 2$ flavor GN model $\equiv$ Fermi-Hubbard model

- A potential model which can be implemented with reconfigurable array of Rydberg atoms in the near future

Continuum Hamiltonian to Lattice Hamiltonian

- Dirac fermion in one spatial dimension:

$$H = \int dx\; i\psi^\dagger \alpha \partial_x \psi + m\psi^\dagger \beta \psi.$$

- Lattice derivatives $\partial \to \Delta_{n'\,n} = \frac{1}{2}\left(\delta_{n'\,n+1} - \delta_{n'\,n-1}\right)$ and redefinition of fields: $\psi(n) \to \alpha^n \lambda(n)$
- Map spinor components to odd and even sites with a choice $\alpha = \sigma_x$.
- With $\beta = \sigma_z$, staggered mass term $m\,(-1)^n\,\lambda^\dagger(n)\lambda(n)$.

$$H = \sum_{n=1}^{L} \Big(\frac{i}{2}\,\lambda^\dagger(n)\left[\lambda(n+1) - \lambda(n-1)\right] + m\,(-1)^n\,\lambda^\dagger(n)\beta\lambda(n) \Big).$$

- Distribute the spinor components on odd and even sites

$$H_0 = \frac{i}{2}\sum_n \chi^\dagger(n)\left[\chi(n+1) - \chi(n-1)\right] + m\sum_n (-1)^n\,\chi^\dagger(n)\chi(n).$$

N-flavor massless Gross-Neveu model

- Free Hamiltonian for N-flavor GN

$$H_0^{(N)} = \overbrace{\frac{i}{2}\sum_n \sum_{a=1}^{N} \chi^{a\dagger}(n)\left[\chi^a(n+1) - \chi^a(n-1)\right]}^{\text{kinetic-term}}$$
$$+ \overbrace{m\,(-1)^n\,\chi^{a\dagger}(n)\chi^a(n)}^{\text{mass-term}}$$

- Four-fermi interaction term for N-flavor GN

$$H_G^{(N)} = -G^2 \sum_n \left(\sum_{a=1}^{N} \chi^{a\dagger}(n)\chi^a(n)\right)^2$$

- $N = 2$ flavor massless case:

$$H_{m=0}^{(2)} = \sum_n \left[\frac{i}{2}\sum_{a=1}^{2} \chi^{a\dagger}(n)\left[\chi^a(n+1) - \chi^a(n-1)\right] - G^2\left(\sum_{a=1}^{N} \chi^{a\dagger}(n)\chi^a(n)\right)^2\right]$$

Jordan-Wigner (JW) transformation

JW transfomration: anticommutation objects (χ) $\longrightarrow$ commutating objects (σ operators)

$$[\chi^{\dagger a}(p), \chi^{b}(q)]_{+} = \delta_{pq}\delta^{ab}$$

$$\left[\sigma_k^a(p), \sigma_\ell^b(q)\right] = 2i\varepsilon_{k\ell m}\sigma_m\delta_{pq}\delta_{ab}$$

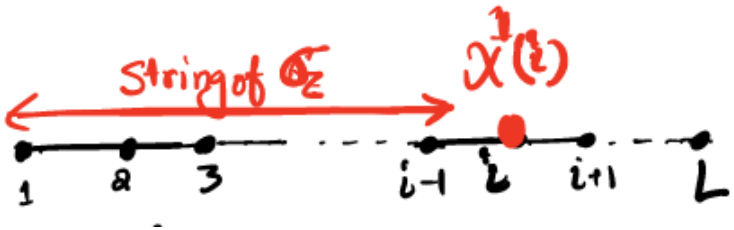
JW transformation

$$\overbrace{\chi^1(i) = P^{(\sigma)}(i-1)\sigma^+(i)}$$

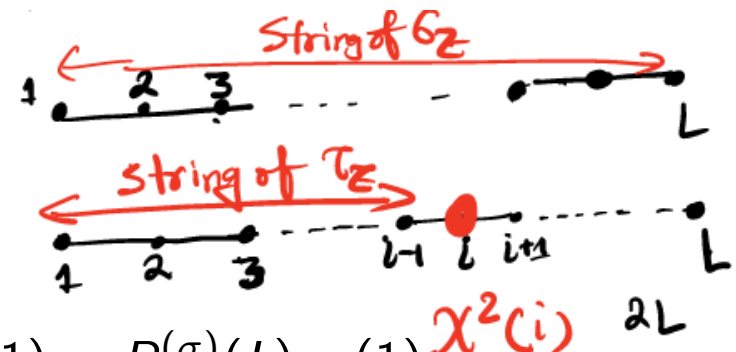
$$\chi^2(i) = P^{(\sigma)}(L)P^{(\tau)}(i-1)\tau^+(i)$$

$$P^{(\sigma)}(i) = \prod_{j=1}^{i}\sigma^z(j)$$

$$P^{(\tau)}(i) = \prod_{j=1}^{i}\tau^z(j)$$



- $\chi^1(1) = \sigma_+(1)$
- $\chi^1(2) = \sigma_z(1)\sigma_+(2)$
- $\chi^1(i) = \sigma_z(1)\sigma_z(2)\cdots\sigma_z(i-1)\sigma_+(i)$
- $P^{(\sigma)}(L) = \sigma_z(1)\sigma_z(2)\cdot\sigma_z(L)$



- $\chi^2(1) = P^{(\sigma)}(L)\tau_+(1)$
- $\chi^2(2) = P^{(\sigma)}(L)\tau_z(1)\tau_+(2)$
- $\chi^2(i) = P^{(\sigma)}(L)\tau_z(1)\tau_z(2)$
$\cdots\tau_z(i-1)\tau_+(i)$

Jordan Wigner-sample calculation

$$\sigma_-\sigma_z = \sigma_- \quad \sigma_+\sigma_z = -\sigma_+ \quad \sigma_z\sigma_- = -\sigma_- \quad \sigma_z\sigma_+ = \sigma_+$$

Now, hopping terms:

$$\begin{aligned}\chi^{\dagger 1}(x)\chi^1(x+1) &= \sigma^-(x)\sigma^3(x-1)\cdots\sigma^3(1)\sigma^3(1)\cdots\sigma^3(x)\sigma^+(x+1)\\ &= \sigma^-(x)\sigma^3(x)\sigma^+(x+1)\\ &= \sigma^-(x)\sigma^+(x+1)\end{aligned}$$

Anti-commutation relations:

$$\begin{aligned}\chi^{\dagger 1}(x)\chi^1(x) &= \sigma^-(x)\sigma^3(x-1)\cdots\sigma^3(1)\sigma^3(1)\cdots\sigma^3(x-1)\sigma^+(x)\\ &= \sigma^-(x)\sigma^+(x)\end{aligned}$$

$$\begin{aligned}\chi^1(x)\chi^{\dagger 1}(x) &= \sigma^3(1)\cdots\sigma^3(x-1)\sigma^+(x)\sigma^-(x)\sigma^3(x-1)\cdots\sigma^3(1)\\ &= \sigma^+(x)\sigma^-(x)\end{aligned}$$

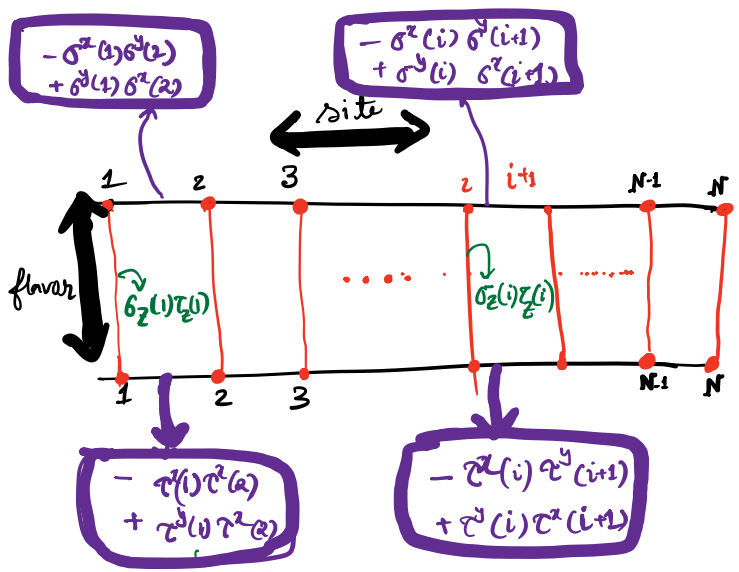
$$[\chi^1(x), \chi^{\dagger 1}(x)]_+ = I$$

Qubit Hamiltonian

Applying open boundary condition

$$H^{(2)} = \frac{1}{2}\sum_{i=1}^{L-1}\Big(-\sigma_x(i)\sigma_y(i+1) + \sigma_y(i)\sigma_x(i+1) - \tau_x(i)\tau_y(i+1) + \tau_y(i)\tau_x(i+1)\Big) + G^2\sum_{i=1}^{L}\Big(\sigma_z(i) + \tau_z(i) + \sigma_z(i)\tau_z(i)\Big)$$

Equivalent to Fermi-Hubbard model $\rightarrow L$ qubits per flavor Reiner *et.el.* 2018



Time evolution of initial state $|\psi\rangle$

- Two non-commutating parts in the Hamiltonian $H^{(N)} = H_{\rm k} + H_{\rm int}$
- Compute $|\langle\psi| \exp(-iHt)|\psi\rangle|^2$ for 2 flavor and 4 flavor GN model with 2 lattice site.
- Trotter approx. $\rightarrow$break time (t) into n discrete steps (δt)

$$\exp(-i\,Ht) = [\exp(-iH_{\rm k}\delta t)\exp(-iH_{\rm int}\delta t)]^n + \mathcal{O}\left(t(\delta t)\right)$$

$$\exp(-iH_{\rm k}\delta t) \sim \exp\left(-i\delta t \sum_{p,f} h_k^f(p)\right) = \exp\left(-i\delta t \sum_{p,f} \sigma_x^f(p)\sigma_y^f(p+1)\right)$$

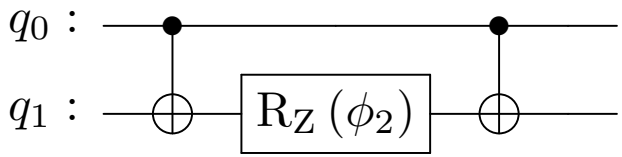
$$= \prod_{p,f} \exp\left(-i\delta t \sigma_x^f(p)\sigma_y^f(p+1)\right) = \prod_{p,f} Q_1^f(p,p+1)$$

$$\exp(-iH_{\rm int}\delta t) \sim \exp\left(-i\delta t \sum_{p} h_{\rm int}(p)\right)$$

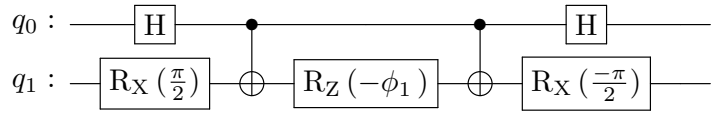
$$= \prod_{p,a\neq b} \exp(-i\delta t\sigma_z^a(p))\exp\left(-i\delta t\sigma_z^b(p)\right)\exp\left(-i\delta t\sigma_z^a(p)\sigma_z^b(p)\right)$$

$$= \prod_{p,a\neq b} R_z^a(p)R_z^b(p)Q_3^{ab}(p,p)$$

Entangling gates: building blocks of the circuit



$$Q_3(q_0, q_1) = \exp\Big(-i\,\frac{\phi_2}{2}\,\sigma_z \otimes \tau_z\Big)$$



$$Q_1(q_0, q_1) = \exp\Big(i\,\frac{\phi_1}{2}\,\sigma_x \otimes \sigma_y\Big)$$

Construction of $Q_3(q_0 = 0, q_1 = 1)$

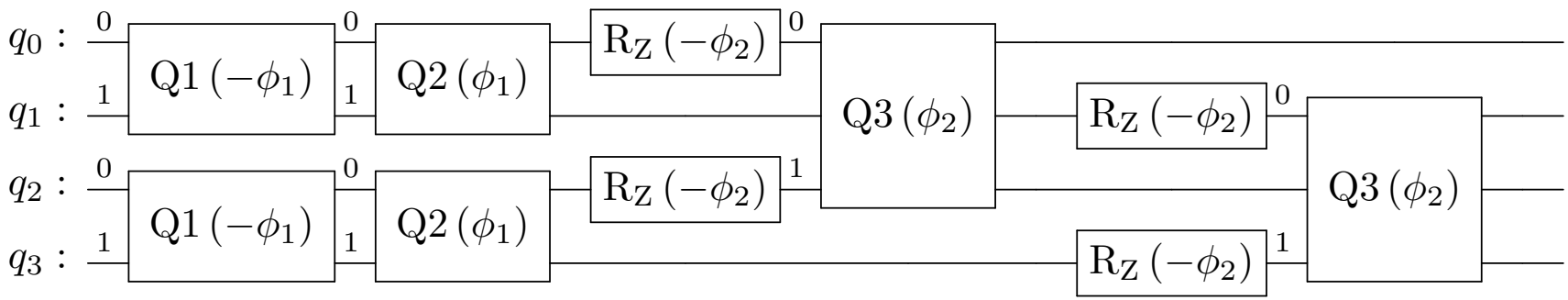
$$\mathrm{CNOT}_{10} = |1\rangle\langle 1| \otimes \sigma_1 + |0\rangle\langle 0| \otimes \mathbf{I}_2.$$

$$(\mathrm{I}_2 \otimes \mathrm{R}_z)\mathrm{CNOT}_{10} = \cos\frac{\phi_2}{2}\,\mathrm{CNOT}_{10} + \sin\frac{\phi_2}{2}(|1\rangle\langle 1| \otimes \sigma_2 + |0\rangle$$

$$\mathrm{R}_z(\phi_2) = \exp\left(-i\frac{\phi_2}{2}\sigma_3\right) = \cos\frac{\phi_2}{2}\,\mathrm{I}_2 - i\,\sin\frac{\phi_2}{2}\,\sigma_3.$$

$$Q_3 = \mathrm{CNOT}_{10}\mathrm{R}_z^1(\phi_2)\mathrm{CNOT}_{10} = \exp\left(-i\,\frac{\phi_2}{2}\,\sigma_z \otimes \tau_z\right)$$

Trotter circuit for two-flavor GN model



Schematic diagram of the Trotter evolution circuit for one trotter step: $N = 2$ flavor, $L = 2$ site, $Q = LN = 4$ qubit case.

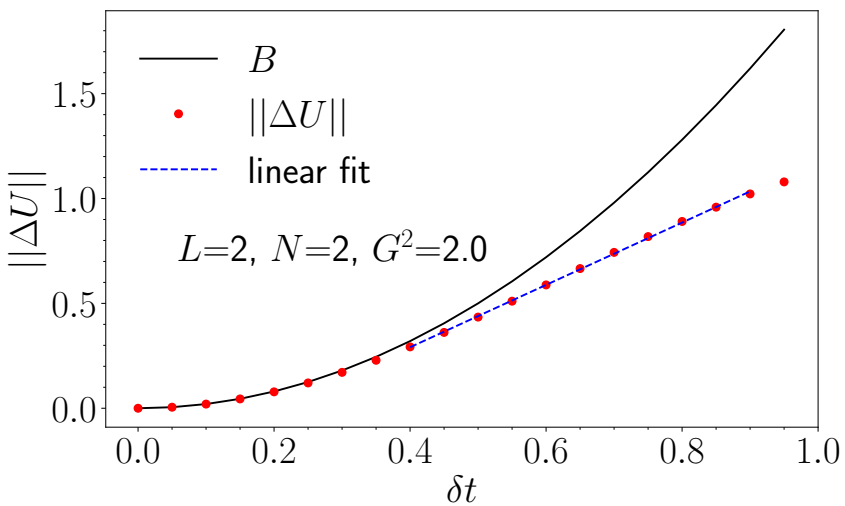
$$\phi_1 = 2\delta t \quad \phi_2 = G^2\delta t$$

Trotter step- how large this can be?

Norm of the following operator determines how large Trotter step can be

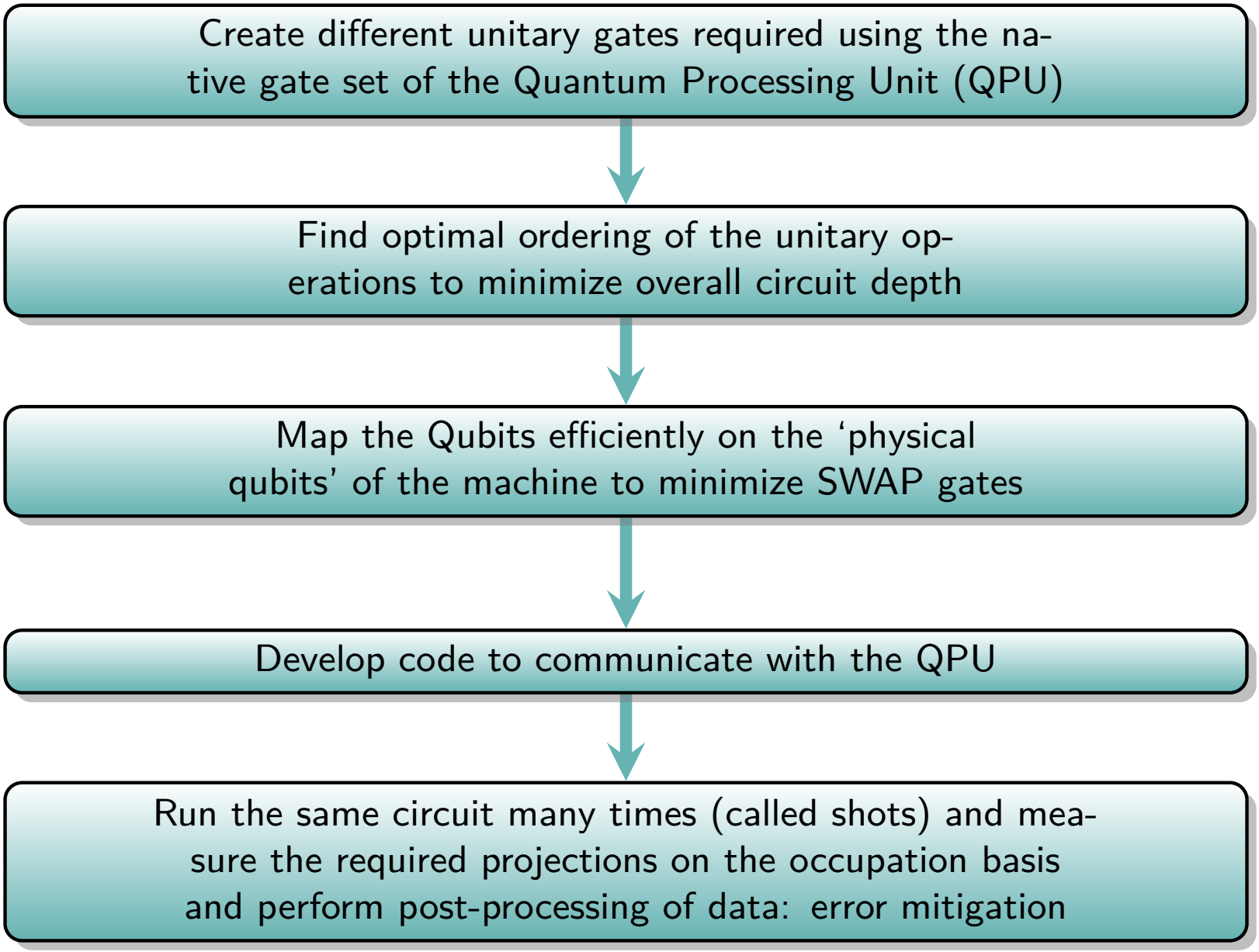
$$\Delta U = \mathrm{e}^{-iH^{(2)}_{m=0}\delta t} - e^{-iH^{(2)}_{0,0}\delta t} e^{-iG^2 H^{(2)}_G \delta t}$$

$$B = (G^2/2)||[H^{(2)}_{0,0}, H^{(2)}_G]||(\delta t)^2$$



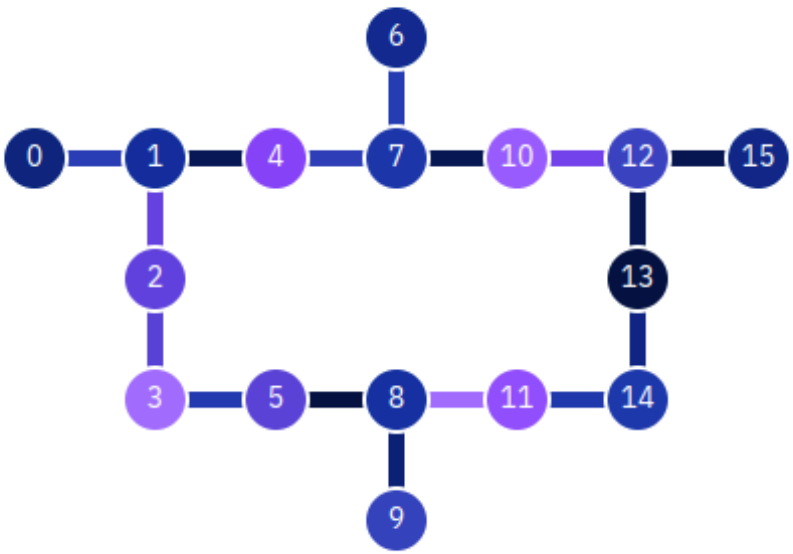
Theoretical bound B for the 1st order Trotter approximation vs. practical bound $||\Delta U||$ computed using matrix exponentiation of our model.

Steps to simulate in quantum processing unit



IBMQ guadalupe

- 16 qubit superconducting quantum computers
- **Fixed topology of qubit connection**
- **Native gate set: CX, ID, RZ, SX, X**

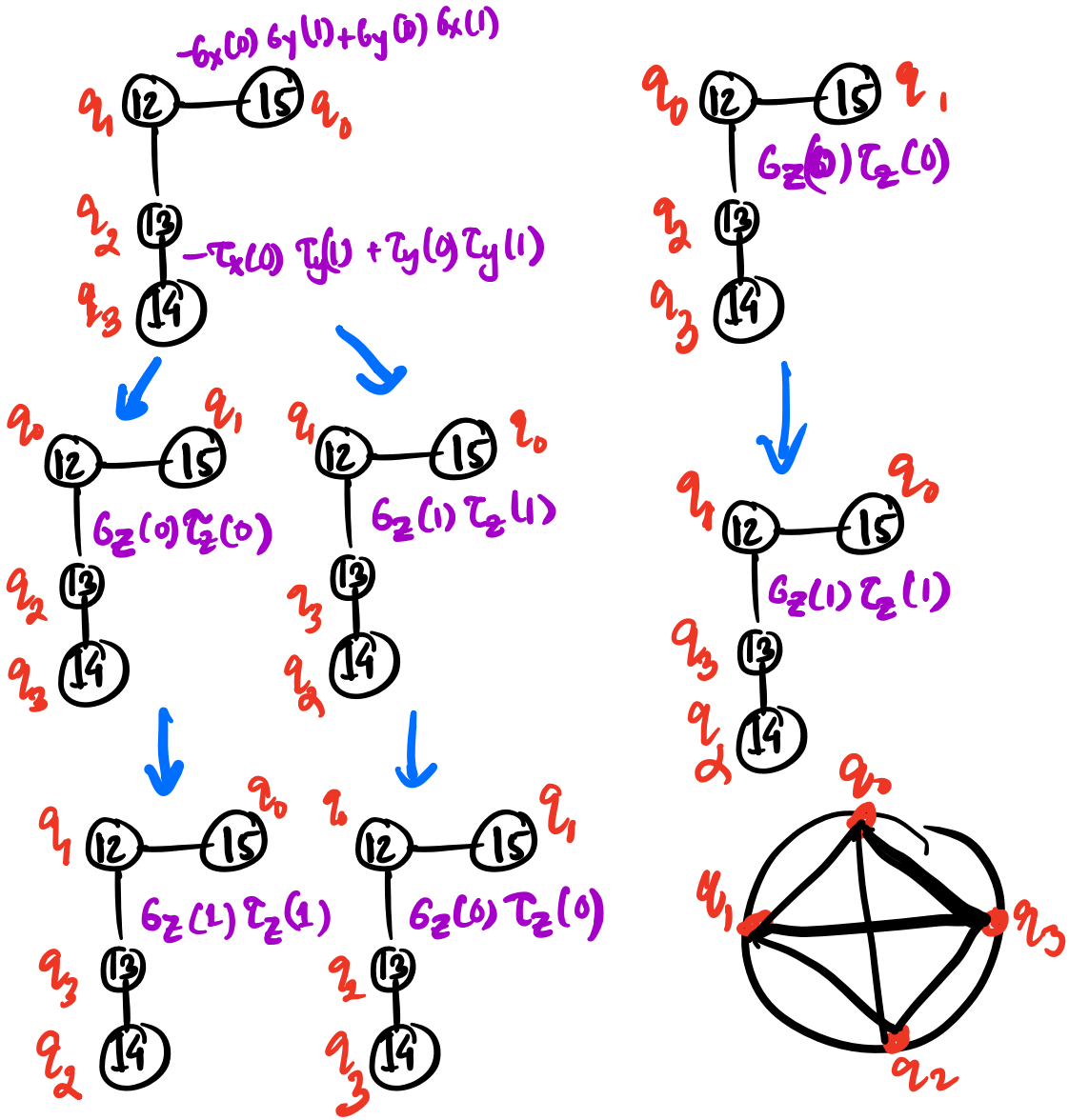


Courtesy: IBMQ experience

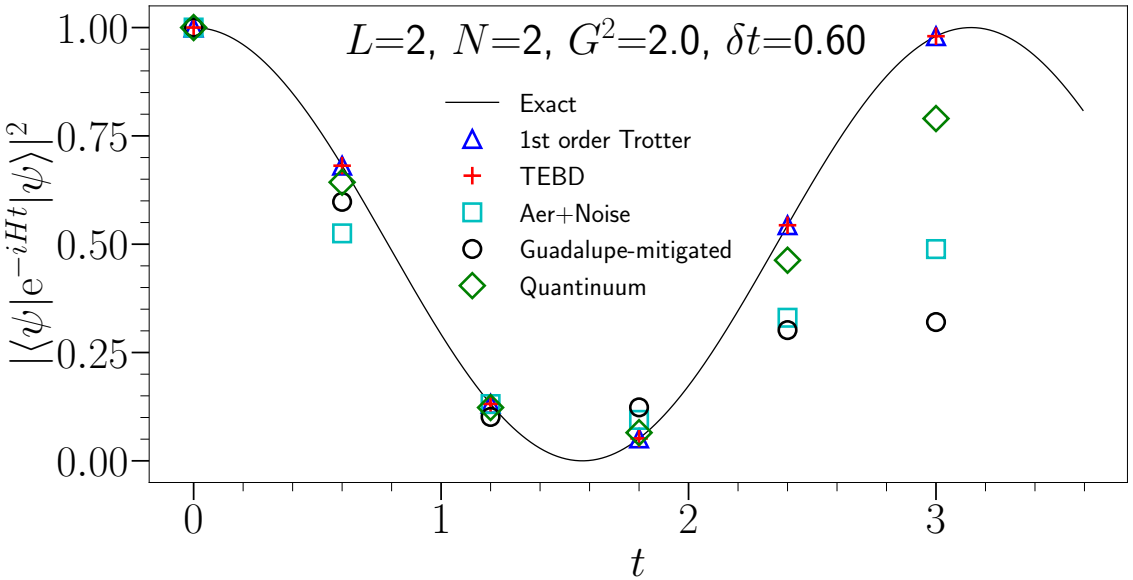
Quantinuum system model H1

- $N \geq 12$ qubit **trapped-ion based quantum computers**
- **All-to-all connectivity**
- Laser based quantum gates
- Quantum charge-coupled device (QCCD) architecture with three or more parallel gate zones in a linear trap
- Mid-circuit measurement conditioned circuit branching
- Qubit reuse after mid-circuit measurement
- **Native gate set: single-qubit rotations, two-qubit ZZ-gates**

Mapping virtual qubits to physical ones

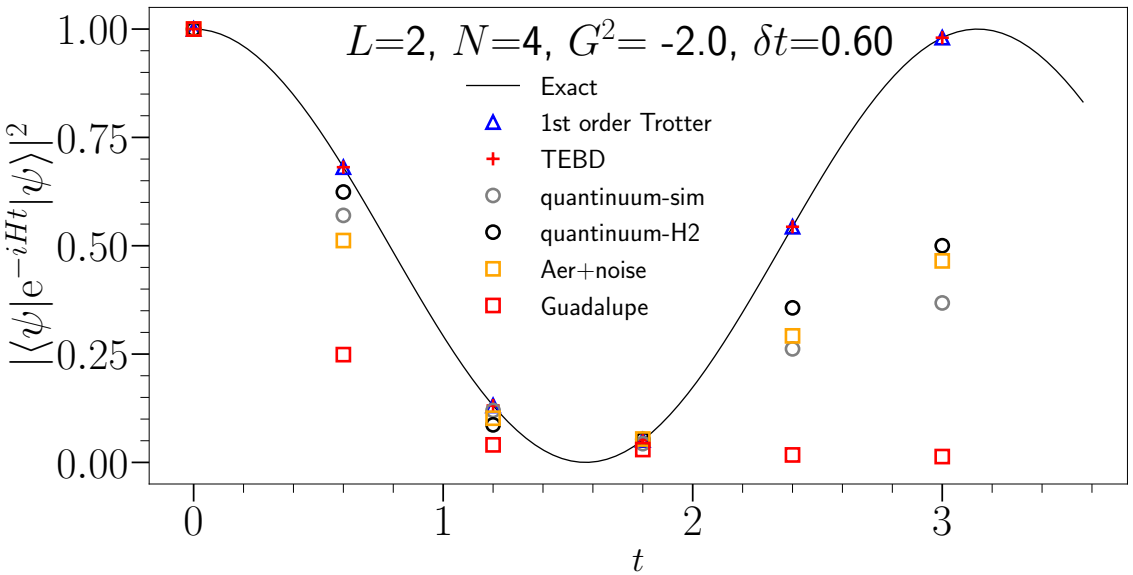


Trotter Evolution: $N = 2$ flavor GN with $L = 2$ lattice site, $|\psi\rangle = |0010\rangle$



		IBMQ		Quantinuum
trotter step, n	d	#2-qubit gates	d	#2-qubit gates
1	12	4	10	4
2	34	18	22	12
3	56	32	34	20
4	78	46	46	28

Trotter evolution: 4 flavor GN with 2 lattice site $|\psi\rangle = |00100000\rangle$



- Quantinuum QPU results outperform IBMQ QPU, especially when all to all connectivity of physical qubits become important when N is larger in our model.
- Quantinuum simulator predicts the Quantinuum QPU results quite well: both in the 4 qubit and 8 qubit case. Device noise model of IBMQ device with Aer simulator predicts data poorly for the 8 qubit case

Ground state preparation-VQE

- the expectation value of the observable H on an arbitrary quantum state $|\psi\rangle$ is given by

$$\langle H\rangle_\psi \equiv \langle\psi|H|\psi\rangle$$

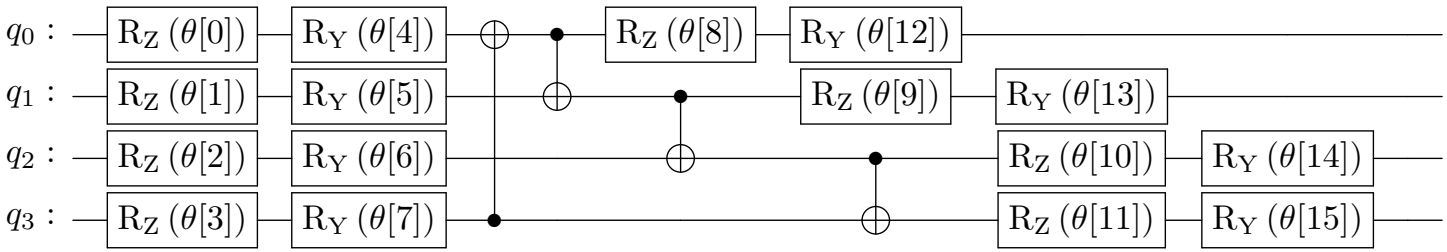
-

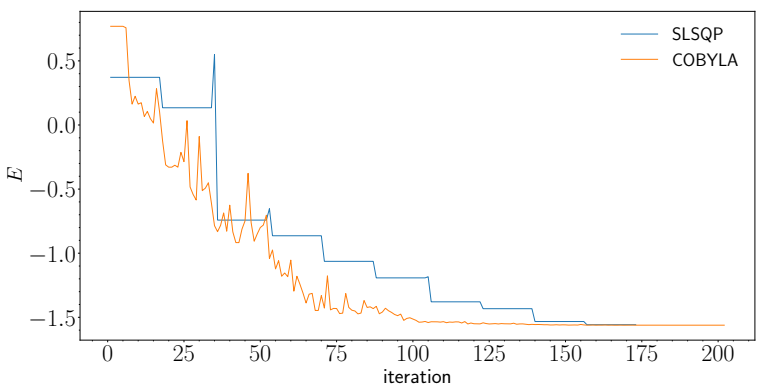
$$E_g \leq \langle H\rangle_\psi = \langle\psi|H|\psi\rangle$$

- Wavefunction of the ground state is presented as a parameterized circuit $U(\theta_1, \cdots, \theta_n)$.
- Parameters are varied at each iteration to minimize $\langle H\rangle_\psi$
- Choice of optimizer can be important to find the real minima

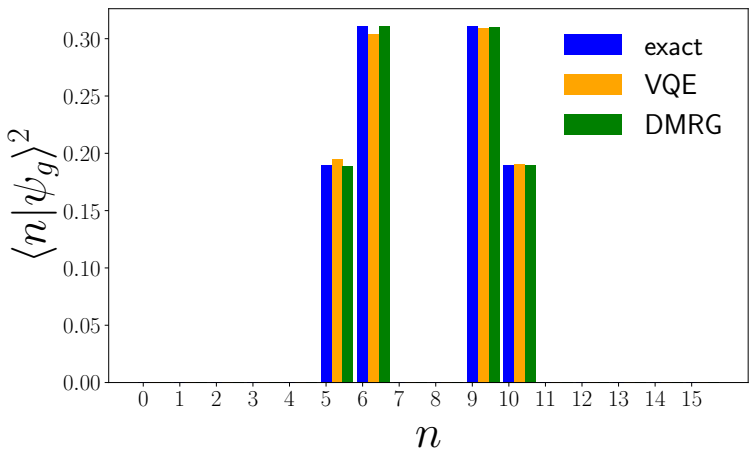
Ground state preperation-VQE: 2 flavor GN

Trial wavefunction $\rightarrow$ Hardware Efficient Approximation (HEA)



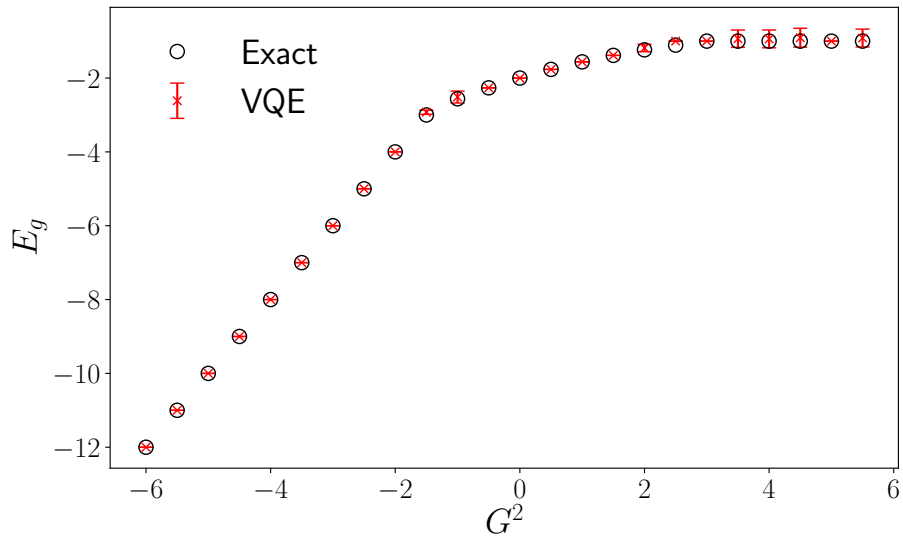


(a) Energy minimization



(b) Projection of ground state of computational basis $|\langle n|\psi_g\rangle|^2$ at $G^2 = 1.0$

Energy spectrum from VQE

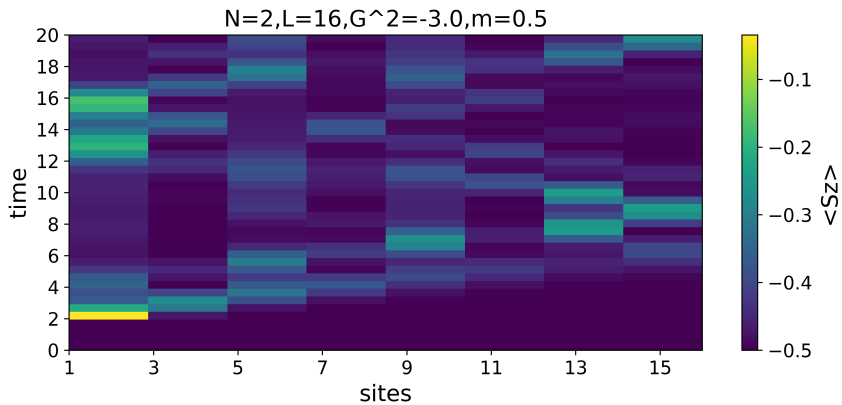


Ground state energy computed from the VQE compared with the results of the exact diagonalization. DMRG results are not shown here as they match exactly with the exact diagonalization result.

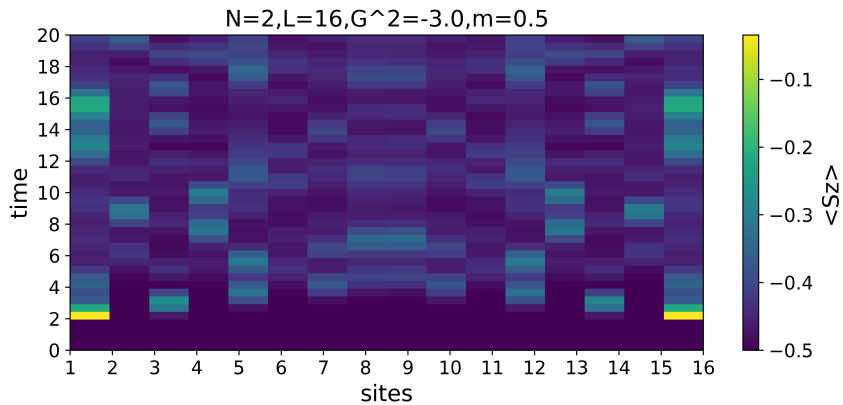
Wave packet preparation and excitation - massive GN model

Jordan-Lee-Preskill prescription for real-time scattering

- Ground state preperation ψ_g (used the MPS form using DMRG)
- Prepare initial wavepacket (used excitaton operator $H_e = e^{ik\sigma^+(x)}\delta(t)$ to find $|\psi_i\rangle = H_e|\psi_g\rangle$)
- Time evolve the excited wavepacket ($|\psi_f\rangle = U_{\text{trotter}}|\psi_i\rangle$)
- measurements of the final state (might require basis transformation in general)



Time evolution for a Right Moving Wave Packet

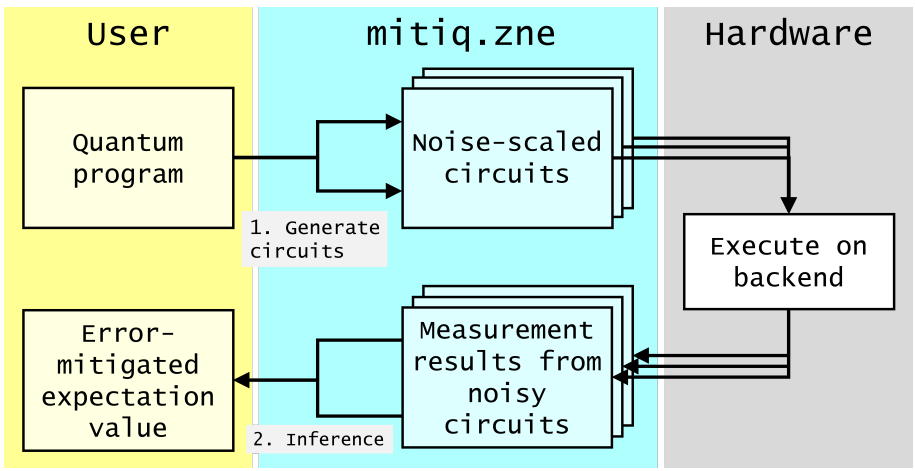


Time evolution for mixed Scattering State

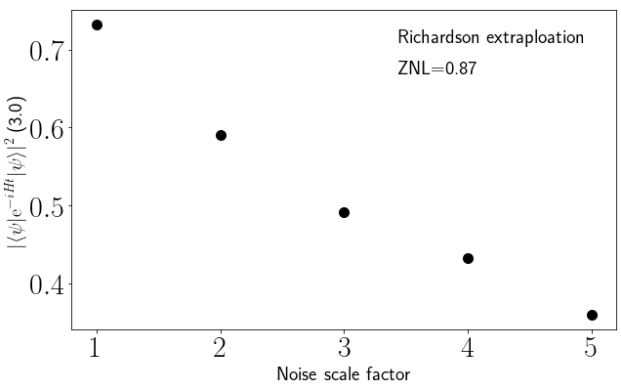
Error mitigation: Zero Noise Extrapolation

- **Why required in NISQ devices?** Error correction scheme is costly
- **What is error mitigation?** Scale noise associated with the circuit to postulate a zero noise limit
- **ZNE steps:** i) noise scaling:
  - unitary gate folding: $G \rightarrow GG^{\dagger}G$
  - pulse stretching : only applicable to devices with pulse-level access

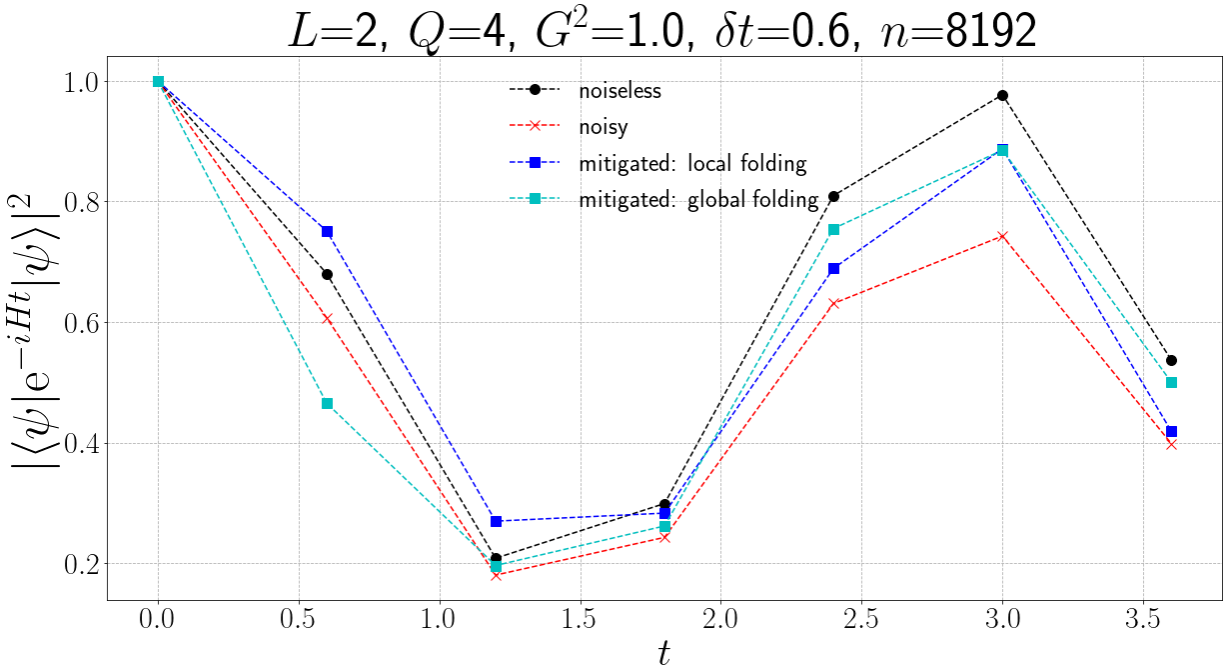
  ii) noise extrapolation: This is performed with a factory object at mitiq



Error mitigation: Zero Noise Extrapolation



Noise scaled expectation value



Trotter Evolution: massless 2 flavor GN model with FakeLima backend

Conclusion

- Time evolution of ground state of a 2-flavor/4-flavor staggered fermionic model with interacting fermions can be realized with NISQ-era machines.
- All-to-all connectivity of the physical qubits proved advantageous for the 4-flavor Trotter evolution.
- Simulation with the noise model of the Honeywell machine indicates that that the ground state can be prepared reliably on the Honeywell quantum processing unit.

Prospects

- Can we scale up the quantum simulation with advanced error mitigation techniques?
- Compute different condensates to probe phase diagram
- Compute entanglement entropy with quantum computers.
- Consider symmetries to reduce circuit depth–essential for computing larger Trotter step computations. Linke *et.el.* 2017
- Improved algorithms to prepare ground state wavefunction. For example adaptive variational eigensolver Harper *et.el.* 2019 or site by site state preperation Jordan*et.el.* 2019

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