

Simulating strongly interacting Hubbard chains with the Variational Hamiltonian Ansatz on a quantum computer

Baptiste Anselme Martin^{1,2} Pascal Simon² Marko J.Rancic¹

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¹TotalEnergies, 8, Boulevard Thomas Gobert – Bât. 861, 91120, Palaiseau

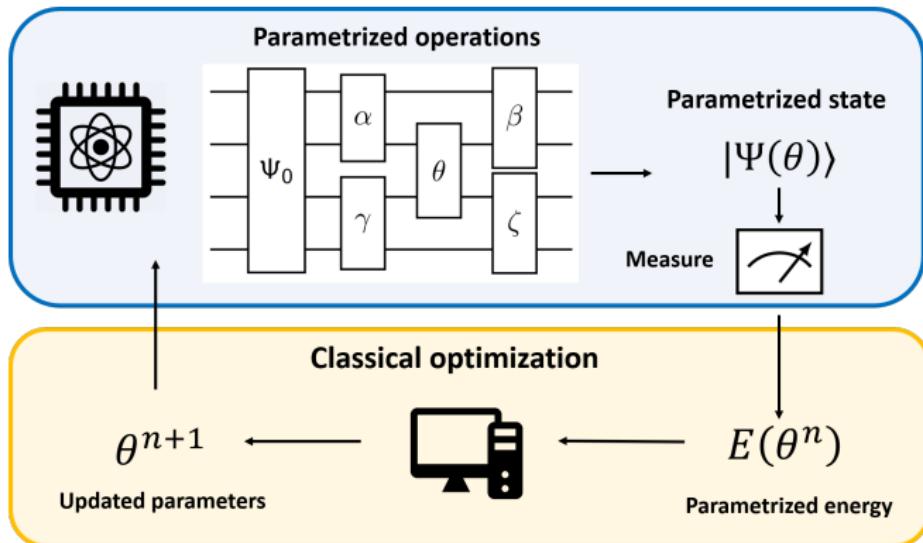
²Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405, Orsay, France

Phys. Rev. Research 4, 023190 (2022)

Variational Quantum Eigensolver (VQE)

Solving variationally a quantum problem :

- $\hat{H} = \sum_i \alpha_i \sigma_i \rightarrow$ groundstate $|\Psi_G\rangle$?
- Guess solution : $|\Psi(\theta)\rangle = \mathcal{U}(\theta) |\Psi_0\rangle$ produced by the quantum computer
- Optimization of θ to minimize $\langle \hat{H} \rangle$



Designing an ansatz

VQE : $|\Psi(\theta)\rangle = \mathcal{U}(\theta) |\Psi_0\rangle$. How to design $|\Psi(\theta)\rangle$?

Hardware efficient

Pros :

- Easy to implement (gate, topology etc)
- Less affected by noise

Cons :

- Less control of the solution
- Scrambling

Ex : RYXXY ansatz

Problem inspired

Pros :

- Physical motivation
- Symmetries etc

Cons :

- Problem specific
- Deep circuit, multiple qubit gates etc

Ex : UCC

→ Variational Hamiltonian Ansatz ?

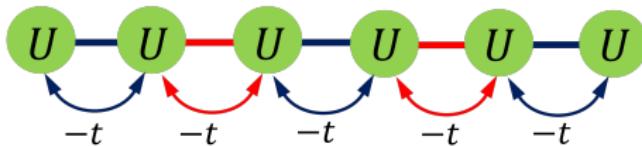
Solving Hubbard model on a quantum computer

Hubbard model

$$H = -t \sum_{i\sigma} \left(c_{i\sigma}^\dagger c_{i+1\sigma} + \text{H.c.} \right) + U \sum_i \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right) \quad (1)$$

hopping *interaction*

$$H = H_t^{(1)} + H_t^{(2)} + H_U$$



$$[H_t, H_U] \neq 0$$

Benchmarks protocols :Pierre-Luc Dallaire-Demers arXiv :2003.01862,
Bryan T. Gard and Adam M. Meier, Phys. Rev. A 105, 042602

First idea

- Prepare free fermion groundstate $|\Psi_0\rangle$
- Adiabatically add interaction H_U to reach groundstate

Adiabatic evolution on quantum computer

Decomposition

$$H = \sum_{\alpha} H^{\alpha}$$
$$[H^{\alpha}, H^{\beta}] \neq 0$$

Trotter-Suzuki approximation

$$e^{A+B} \simeq e^A e^B$$

Approximation for time-evolution operator

$$e^{-i \int H(\tau) d\tau} \simeq \prod_n^n e^{-i H_t \Delta \tau - i H_U \frac{n}{N} \Delta \tau}$$
$$\simeq \prod_n^n e^{-i H_t^{(1)} \Delta \tau} e^{-i H_t^{(2)} \Delta \tau} e^{-i H_U \frac{n}{N} \Delta \tau}$$

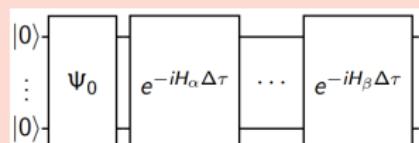
Fermion-to-qubit mapping

$$e^{-ih\theta} \rightarrow e^{-i\sigma\theta}$$

h : fermion operator
 σ : Pauli strings

Gate decomposition

Quantum circuit



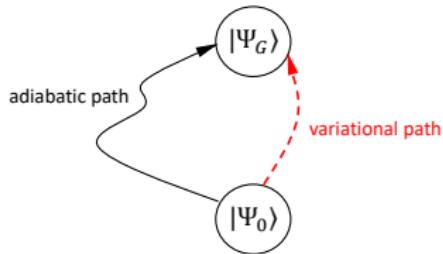
$$|\Psi(t)\rangle \simeq \prod_{n=1}^N e^{-i H_t^{(1)} \Delta \tau} e^{-i H_t^{(2)} \Delta \tau} e^{-i H_U \Delta \tau \frac{n}{N}} |\Psi_0\rangle \quad (2)$$

From adiabatic evolution to Variational Hamiltonian Ansatz

Idea :

time step $\Delta\tau \rightarrow$ variational parameters θ

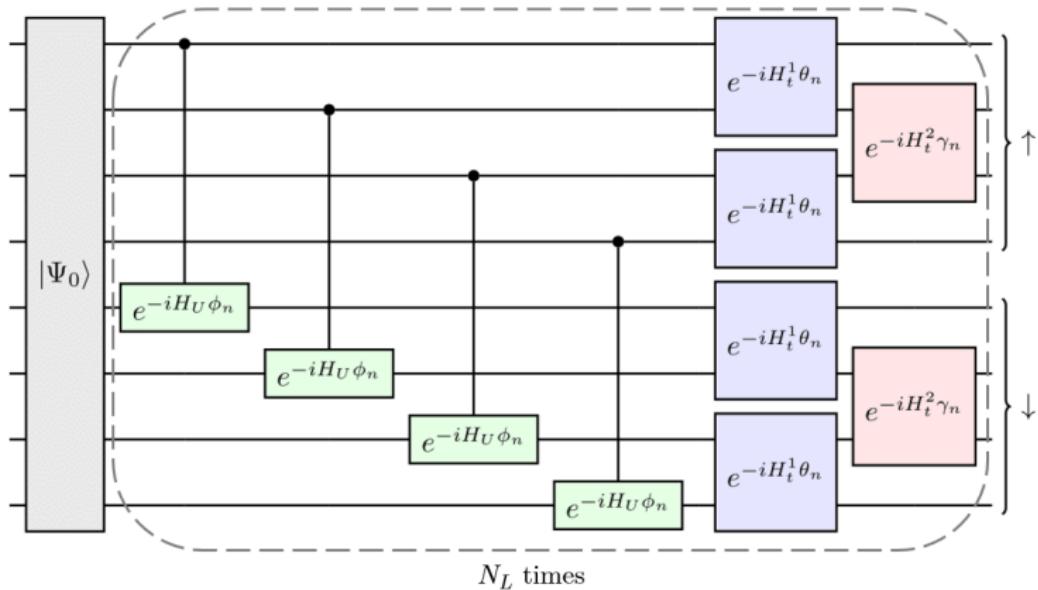
- Reduced circuit length
- Hope to find optimized path to the groundstate
- Proposed by : D. Wecker, M. B. Hastings, and M. Troyer Phys. Rev. A 92, 042303



Variational circuit

$$|\Psi(\theta)\rangle = \prod_{n=1}^{N_L} e^{-iH_t^{(1)}\theta_n^1} e^{-iH_t^{(2)}\theta_n^2} e^{-iH_U\theta_n^U} |\Psi_0\rangle \quad (3)$$

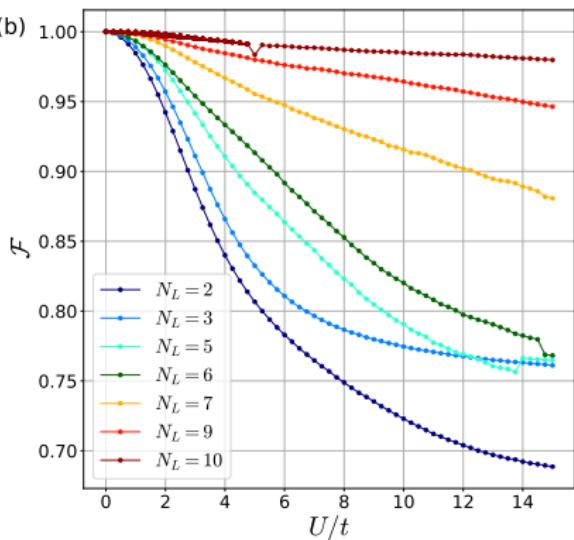
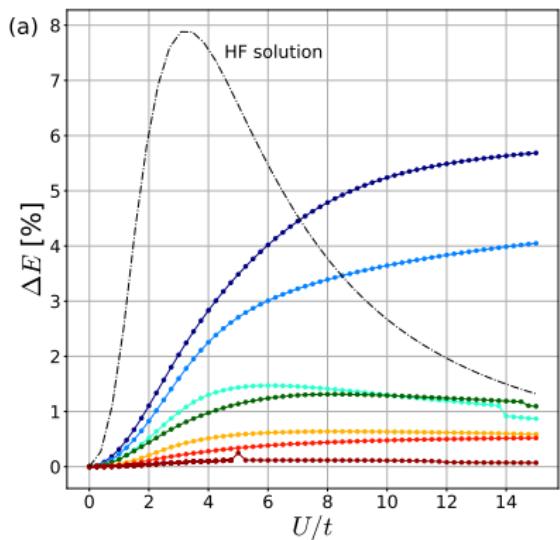
Variational circuit



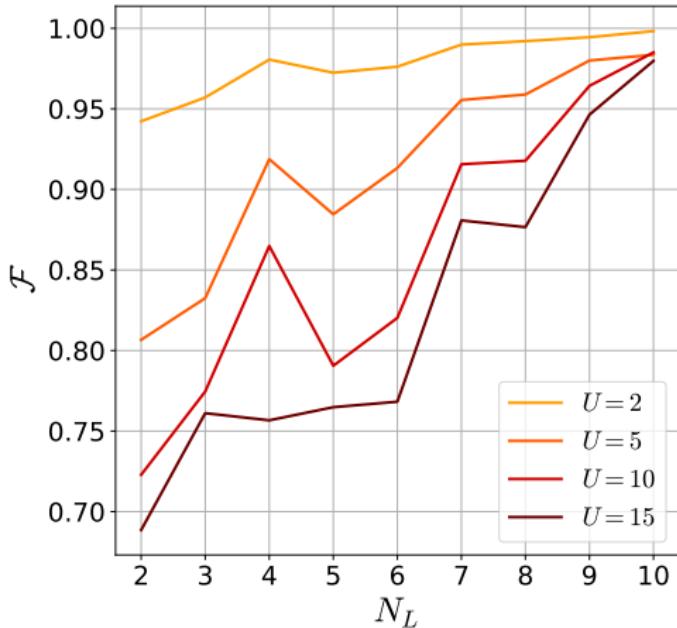
$$|\Psi(\theta)\rangle = \prod_{n=1}^{N_L} e^{-iH_t^{(1)}\theta_n^1} e^{-iH_t^{(2)}\theta_n^2} e^{-iH_U\theta_n^U} |\Psi_0\rangle$$

Results for 8 site Hubbard chain : Phys. Rev. Research 4, 023190

- Previous work : C.Cade et al, Phys. Rev. B 102 (2020)
- VQE algorithm simulation performed on Atos Quantum Learning Machine
- Initial state prepared with OpenFermion : J.R. McClean, Quantum Science and Technology 5.3 (2020) : 034014
- COBYLA optimizer

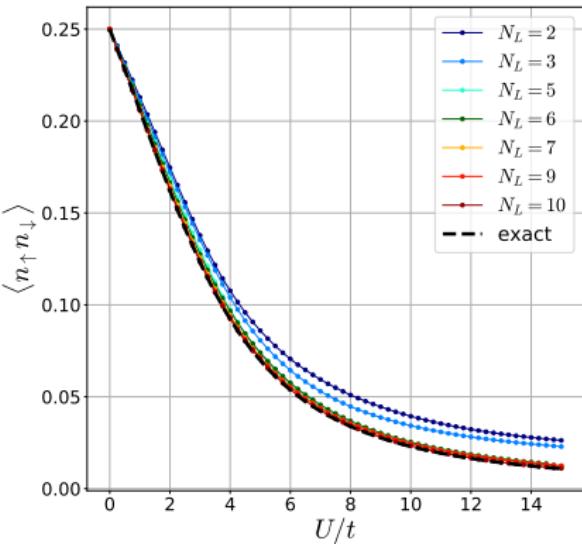
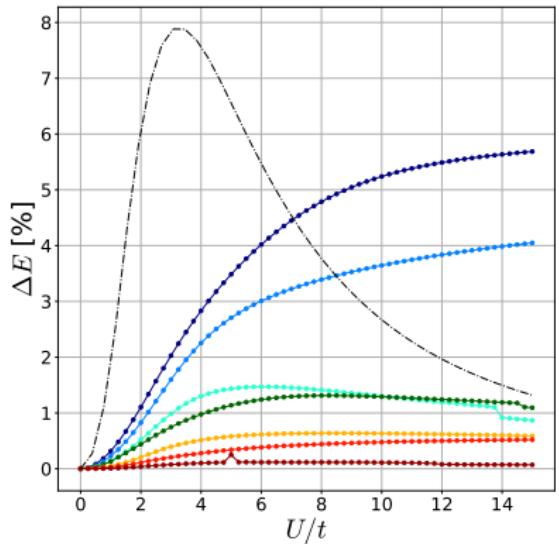


Results for 8 sites Hubbard chain



- $N_L \nearrow$: better fidelity most of the time
- $U/t \gg 1$: groundstates harder to reach

What physics can we get ?

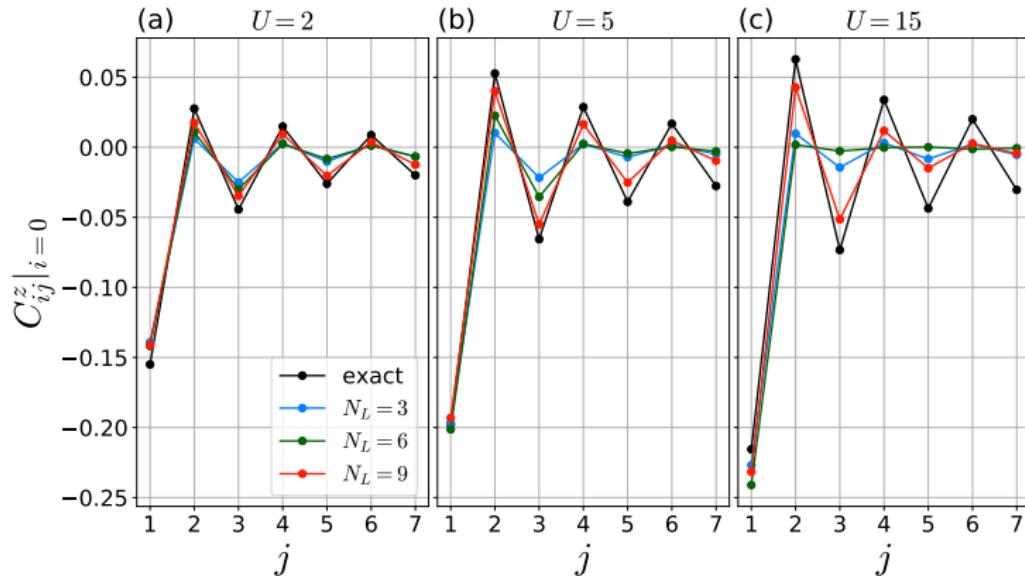


⇒ We still see electron localization as $U \nearrow$ even for low N_L

Spin correlation ?

We expect antiferromagnetic order, do we see it ?

$$C_{ij}^z = \langle S_i^z S_j^z \rangle - \langle S_i^z \rangle \langle S_j^z \rangle$$

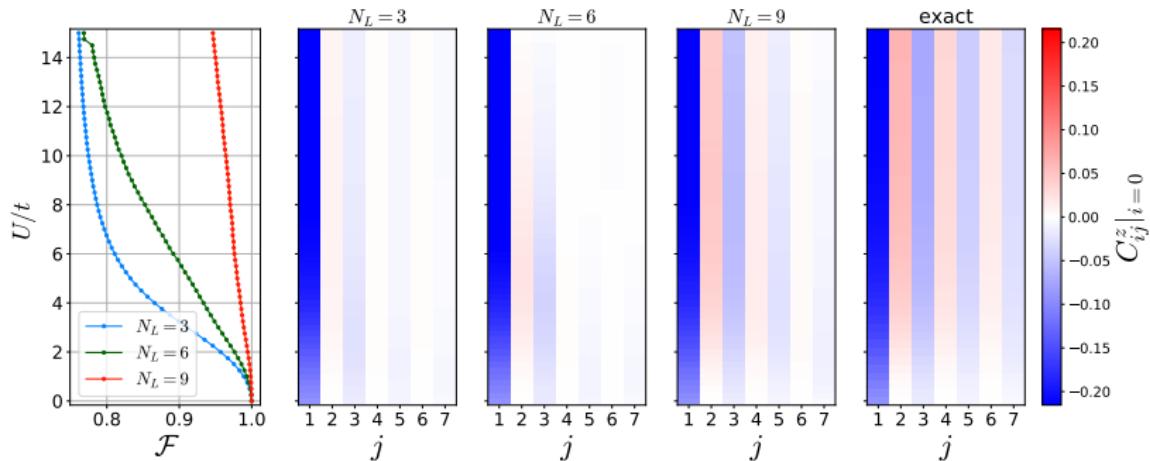


→ For large U , correlations hard to capture, need for large N_L

Spin correlation ?

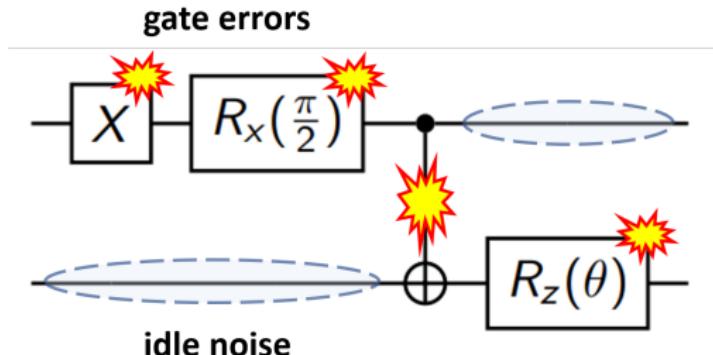
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What about noise ?



- : Phase and Amplitude damping T_1 and T_2
- : Faulty gates $\rho' = \sum_k K_k \rho K_k^\dagger$

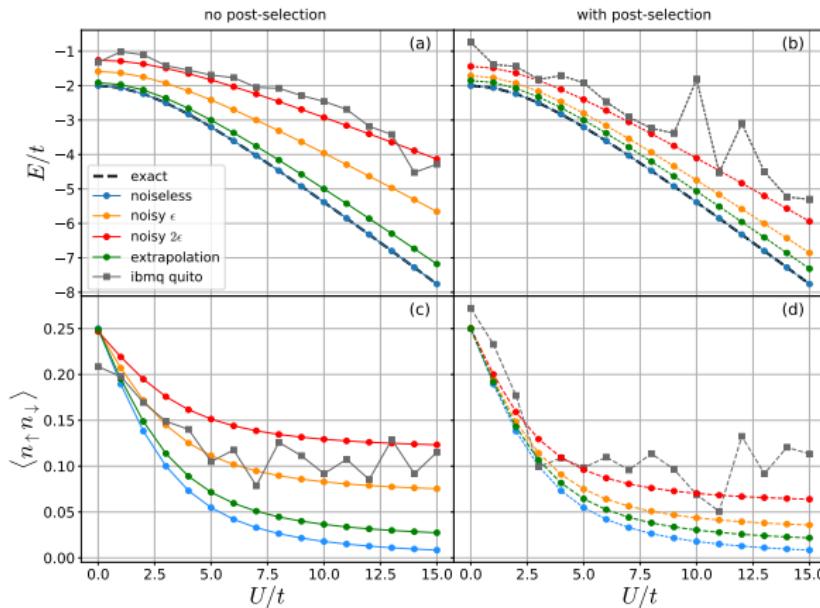
$$K_0 = \sqrt{1-p}I, K_1 = \sqrt{\frac{p}{3}}X, K_2 = \sqrt{\frac{p}{3}}Y, K_3 = \sqrt{\frac{p}{3}}Z$$

$p \sim \epsilon$, with ϵ = gate's error rate

Noisy simulations and experiment : 2 site Hubbard model

Density matrix calculation with noise models and error mitigation

- Richardson extrapolation : $\langle \hat{O} \rangle = O^* + \sum_k c_k \epsilon^k \simeq O^* + c_1 \epsilon$
[Kandala et al. Nature 567, 491–495 (2019)]
- Post-selection based on N and S^z symmetries
- Experimental data from `ibmq_quito`



Conclusion

Variational Hamiltonian Ansatz for strongly interacting Hubbard chains : how does it perform ?

Quantity	Low depth	High depth
Energy E	✓	✓
Fidelity \mathcal{F}	✗	✓
local correlators	✓	✓
long range correlators	✗	✓
noise	~*	✗



B. Anselme Martin, P. Simon, M. J. Rancic, Phys. Rev. Research 4, 023190 (2022)

* S. Stanisic et al, Nat Commun 13, 5743 (2022).