Title: Strategies for solving the Fermi-Hubbard model on near-term quantum computers

Speakers: Ashley Montanaro

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Abstract: The Fermi-Hubbard model is of fundamental importance in condensed-matter physics, yet is extremely challenging to solve numerically. Finding the ground state of the Hubbard model using variational methods has been predicted to be one of the first applications of near-term quantum computers. In this talk, I will discuss recent work which carried out a detailed analysis and optimisation of the complexity of variational quantum algorithms for finding the ground state of the Hubbard model, including extensive numerical experiments for systems with up to 12 sites. The depth complexities we find are substantially lower than previous work. If our numerical results on small lattice sizes are representative of the somewhat larger lattices accessible to near-term quantum hardware, they suggest that optimising over quantum circuits with a gate depth less than a thousand could be sufficient to solve instances of the Hubbard model beyond the capacity of classical exact diagonalisation. I will also discuss a proof-of-principle implementation on Rigetti quantum computing hardware.

The talk is based on joint work with Chris Cade, Lana Mineh and Stasja Stanisic (arXiv:1912.06007 , arXiv:2006.01179).

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University of BRISTOL

STRATEGIES FOR SOLVING THE FERMI-HUBBARD MODEL ON NEAR-TERM QUANTUM COMPUTERS

Ashley Montanaro
Joint work with Chris Cade, Lana Mineh and Stasja Stanisic

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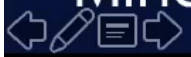
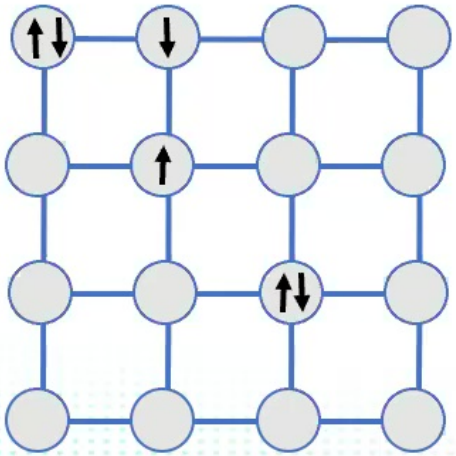


The Fermi-Hubbard model

An iconic model in condensed-matter physics for strongly correlated electronic systems

Predicted to be one of the first targets for quantum computers in the NISQ era



$$H = -t \sum_{\langle i,j \rangle, \sigma} (a^\dagger_{i\sigma} a_{j\sigma} + a^\dagger_{j\sigma} a_{i\sigma}) + U \sum_k n_{k\uparrow} n_{k\downarrow}$$

Hopping term

Onsite term

Task: find the ground state of H

Exact solution of a Hubbard model instance with 17 fermions on 22 sites required 7TB of memory and 13 TFlops (Yamada et al '05)

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Variational Quantum Eigensolver (VQE)

The VQE approach tries to find the ground state of a Hamiltonian H by optimising over quantum circuits to minimise the energy of the state produced with respect to H

We need to make many decisions about the algorithm:

1. How to represent H on a quantum computer?
2. What family of circuits ("ansatz") to optimise over?
3. How to implement the circuits efficiently?
4. Which classical optimisation algorithm to use?

Here we make choices for each of these; calculate the complexity in detail; and carry out numerical experiments to determine how well the algorithm will perform.

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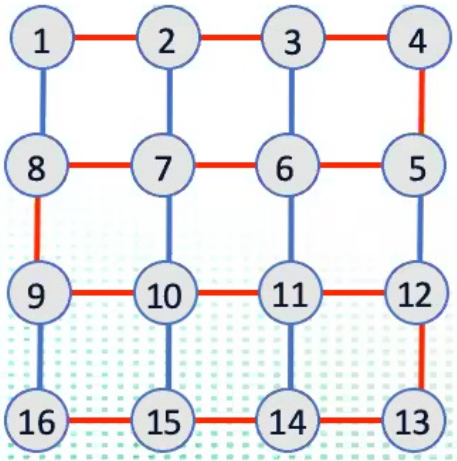
Representing the Hubbard model

We use the **Jordan-Wigner** transform, which associates each site and spin-type with 1 qubit

An n_x x n_y lattice requires $2n_xn_y$ qubits

$$a_j^\dagger a_k + a_k^\dagger a_j \mapsto \frac{1}{2}(X_j X_k + Y_j Y_k) Z_{j+1} \cdots Z_{k-1}$$

$$a_j^\dagger a_j a_k^\dagger a_k \mapsto \frac{1}{4}(I - Z_j)(I - Z_k)$$



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Variational ansatz

We use the **Hamiltonian Variational** ansatz (Wecker et al '15)

- Splits the Hamiltonian into commuting terms (horizontal x2, vertical x2, onsite)
- Starts in the ground state of the noninteracting Hamiltonian (U=0)
  - Can be efficiently prepared using Givens rotations (Kivlichan et al '18) in depth $n_x n_y$ - 1
- Alternates layers of time-evolution according to different terms, for different times
- Each layer is of the form

$$e^{itV_2}H_{V_2}\,e^{itH_2}H_{H_2}\,e^{itV_1}H_{V_1}\,e^{itH_1}H_{H_1}\,e^{itH_O}H_O$$

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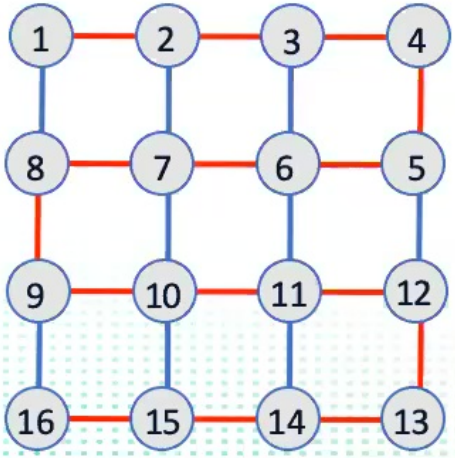
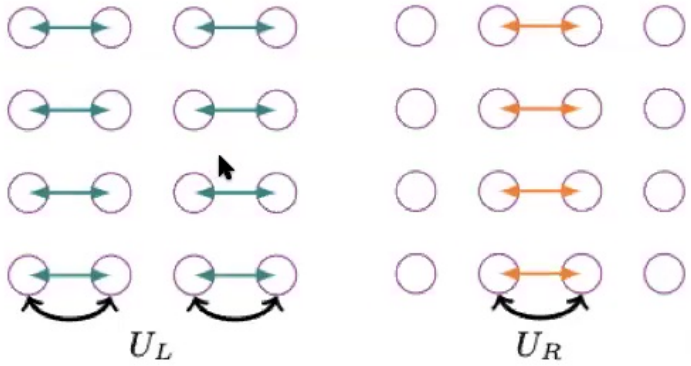
Efficient implementation

To help with the long Jordan-Wigner strings, we use fermionic swap networks (Kivlichan et al '18)

These effectively rearrange the Jordan-Wigner ordering, allowing us to implement all of the vertical hopping terms relatively efficiently





$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

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Efficient implementation

The final 2-qubit gate depth to implement one layer of all required interactions is:

Architecture	Ansatz circuit depth per layer
Fully Connected	$\mathbf{2n_x + 1 \,/\, 2n_x + 2}$ $4 \times 4 \,/\, 4 \times 5 : 9$ $5 \times 5 \,/\, 5 \times 6 : 12$ $6 \times 6 : 13$
Nearest Neighbour	$\mathbf{4n_x + 1 \,/\, 4n_x + 2}$ $4 \times 4 \,/\, 4 \times 5 : 17$ $5 \times 5 \,/\, 5 \times 6 : 22$ $6 \times 6 : 25$
Google Sycamore	$\mathbf{6n_x + 1 \,/\, 6n_x + 2}$ $4 \times 4 \,/\, 4 \times 5 : 25$ $5 \times 5 \,/\, 5 \times 6 : 32$ $6 \times 6 : 37$

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Number preserving ansatz

Now all the gates that occur in the quantum circuit are of the form

$$U_{\mathrm{NP}}(\theta,\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & i\sin\theta & 0 \\ 0 & i\sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix}$$

- In the Hamiltonian Variational ansatz, the parameters have relationships between each other - we have at most 5 independent parameters per layer
- But we can also allow all the parameters to be independent
- We call this the Number Preserving ansatz

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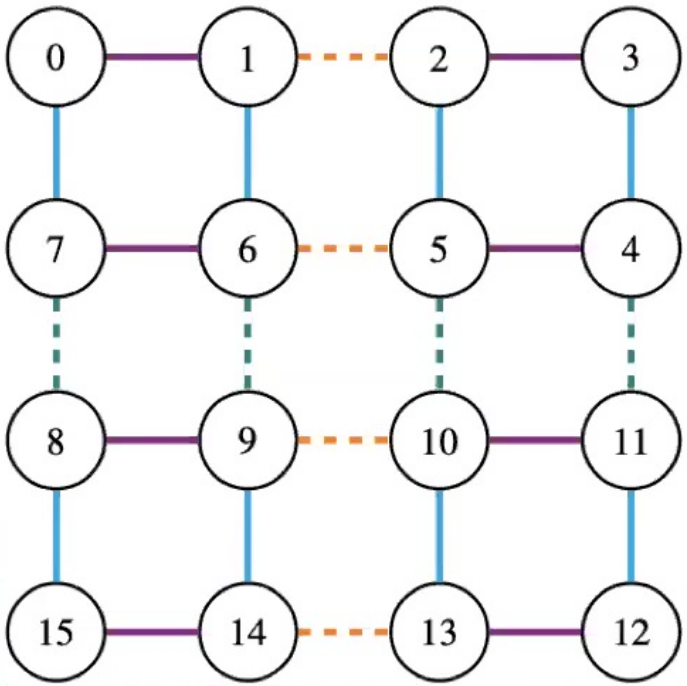
Efficient implementation



Next, we need to measure the energy of the states produced efficiently

We can do this by splitting the hopping terms into 4 commuting parts, and measuring all the terms in each commuting part simultaneously

To achieve high accuracy in the energy estimate then needs many measurements (e.g. error 0.01 -> ~10^3 measurements)

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Classical optimisation algorithm

Finally, we need to decide what method to use for classical optimisation over quantum circuits

Many optimisation techniques don't work if we use realistic measurements because of statistical noise

Two methods that do work:

- Simultaneous Perturbation Stochastic Approximation (SPSA)
  - "Gradient descent along a random line"

- Coordinate descent (CD)
  - aka sequential minimal optimisation (Nakanishi et al '19), Rotosolve (Ostaszewski et al '19), Jacobi diagonalisation (Parrish et al '19), ...
  - Uses polynomial interpolation to exactly minimise the energy in terms of one parameter at a time

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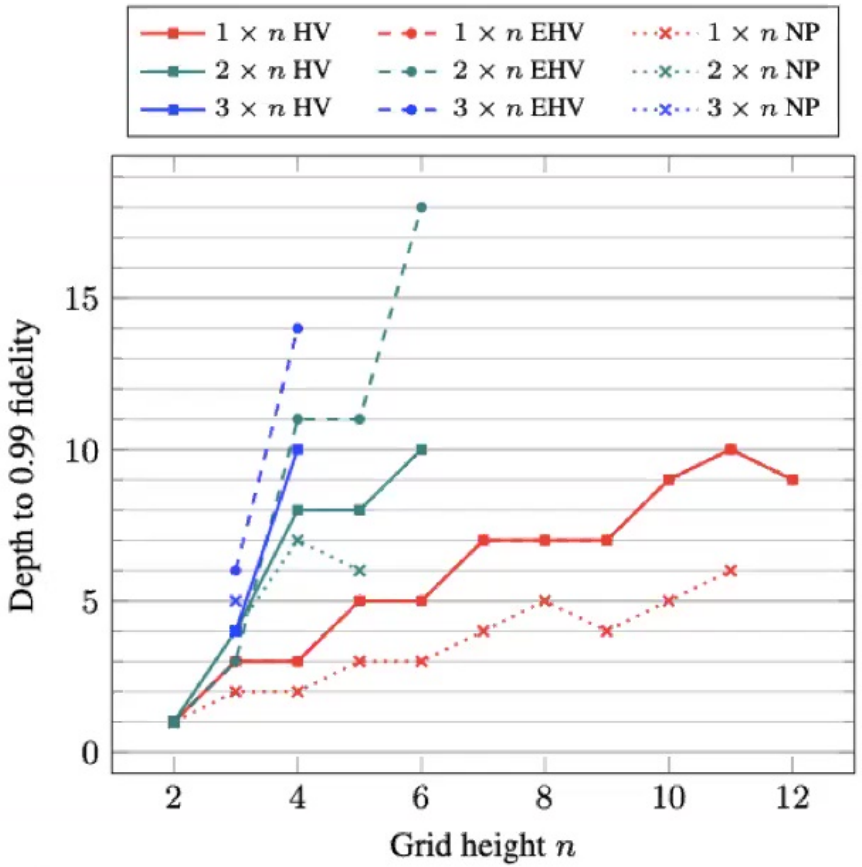
Numerical results

We evaluated the performance of VQE on systems up to 12 sites (24 qubits) in classical simulation

First: ability of the variational ansatz to produce the ground state under optimal conditions

- Exact energy measurements, BFGS optimiser

Our results are consistent with a system with N sites needing ~N layers of the variational circuit



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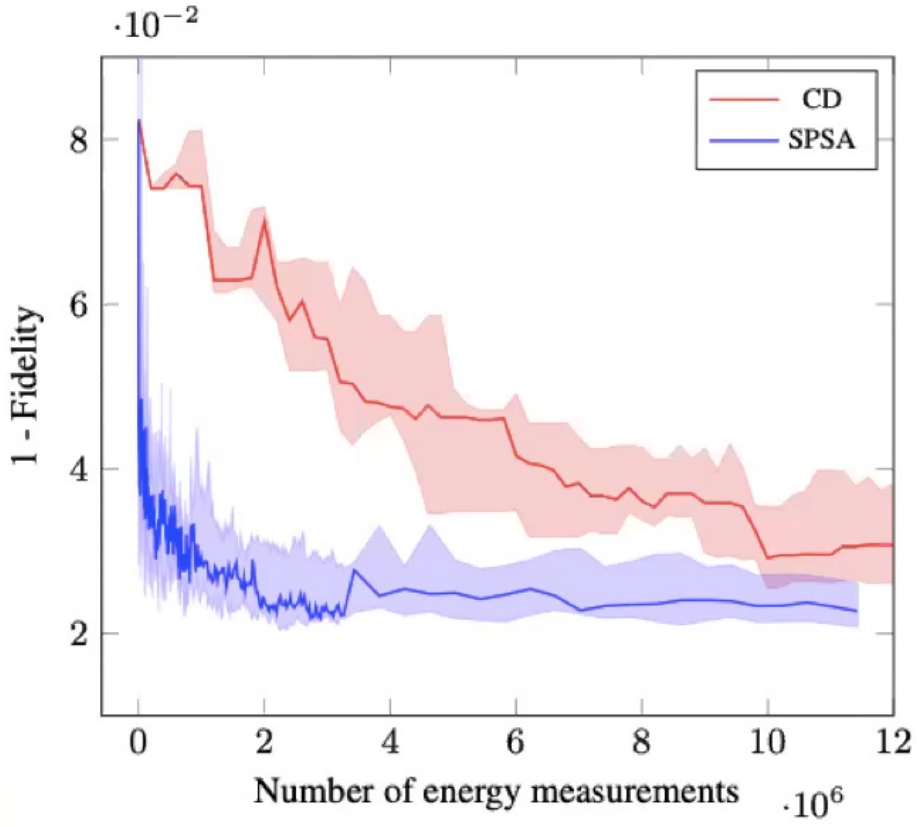
Numerical results

Second: ability of the optimiser to find the ground state with realistic measurements, incorporating statistical noise

Graph shows a 3x3 lattice with CD and SPSA algorithms



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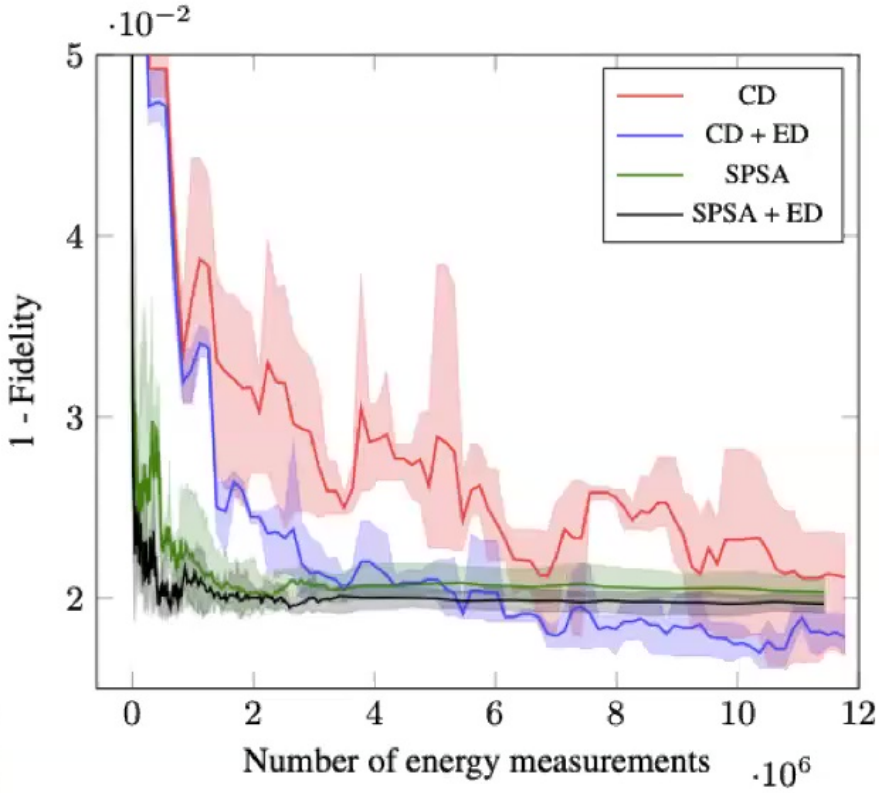
Numerical results

Third: effect of errors in the quantum circuit

Figure shows a 2x3 lattice with 10^{-3} depolarising noise, including the effect of error detection by checking occupation number



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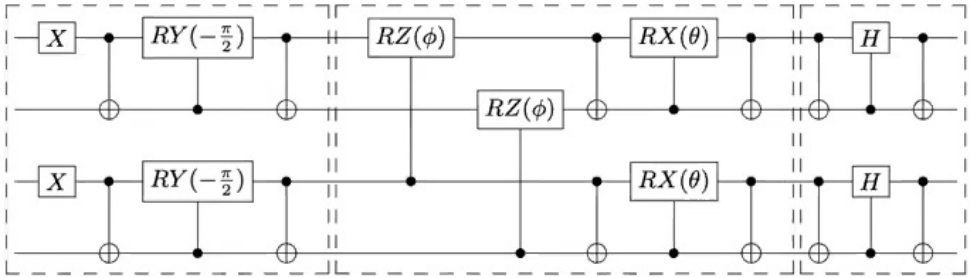
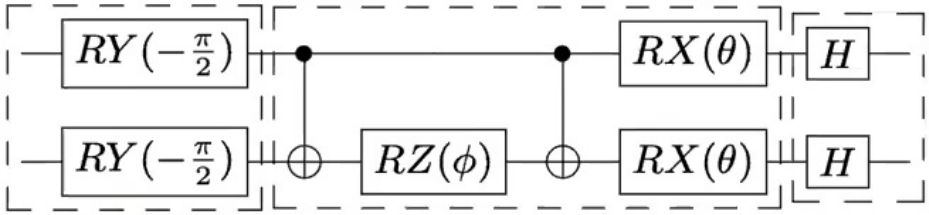
Experimental implementation

We implemented VQE for the simplest nontrivial case of the Hubbard model (2x1) on Rigetti Aspen-4 and Aspen-7 quantum hardware



As well as the standard implementation discussed above (4 qubits), we considered a compressed implementation on 2 qubits

Compression uses that the Hubbard Hamiltonian preserves occupation number for each spin-type



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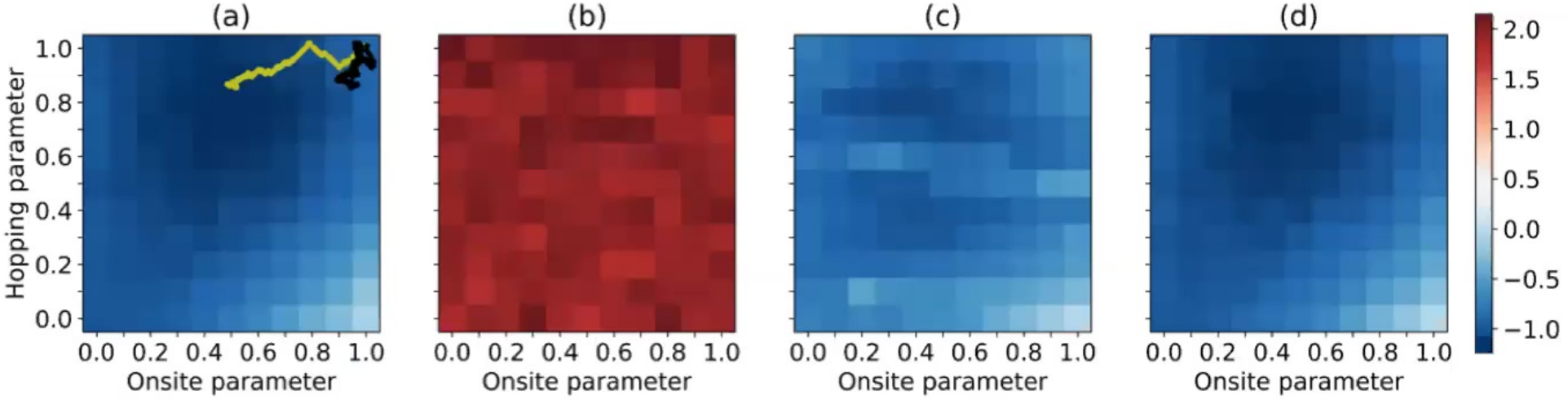
Experimental results

Heatmaps showing the performance of the algorithm:



Classical simulation

Uncompressed, Aspen-7

Compressed, Aspen-7

Compressed, Aspen-4

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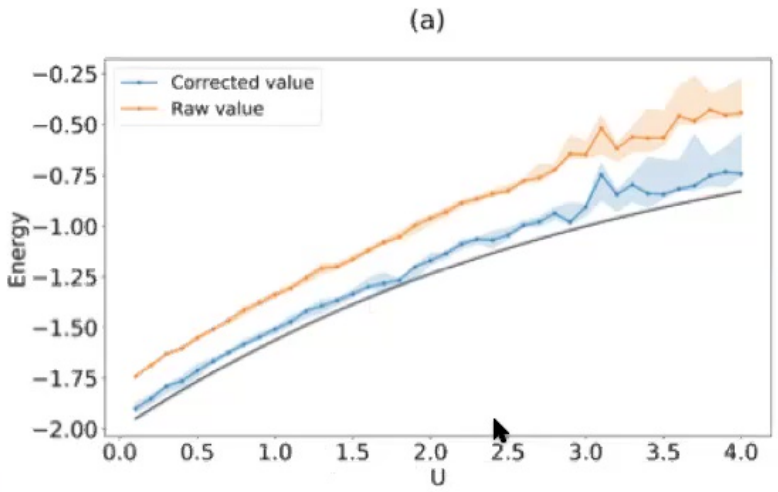
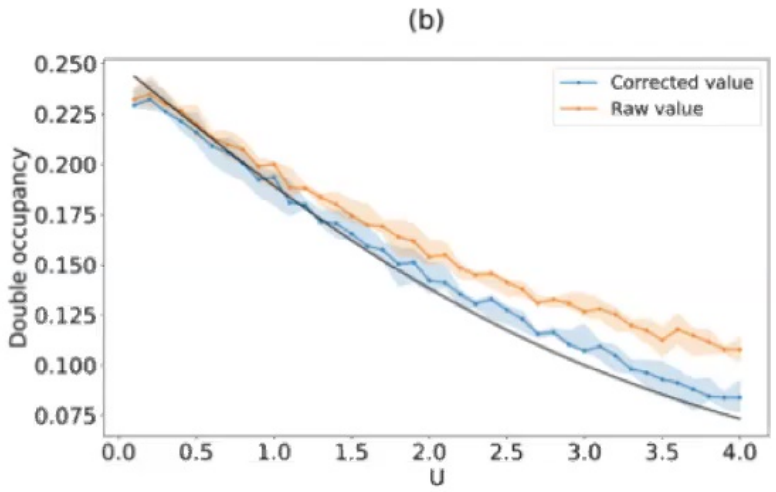
Experimental results

Extracting physically meaningful results from the ground state:



Ground state energy



Double occupancy

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Conclusions

The VQE approach can find ground states of small instances of the Hubbard model efficiently

If these results are representative of the situation for larger systems, the ground state of a **5x5** Hubbard instance (beyond the capacity of classical exact diagonalisation) could be found with quantum circuits of 2-qubit gate depth **<400** (in a fully-connected architecture)

The algorithm works when implemented on a small quantum computer and can produce physically meaningful results...

Though there's still a long way to go before we outperform classical methods!

Further reading

arXiv:1912.06007 (Phys. Rev. B, to appear)
arXiv:2006.01179

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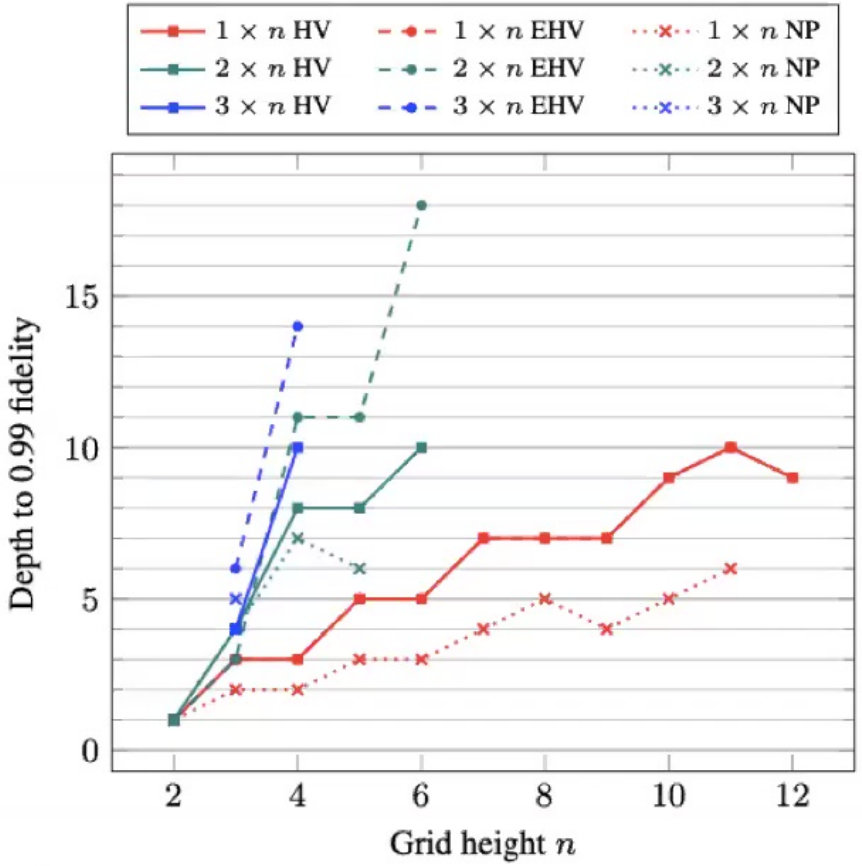

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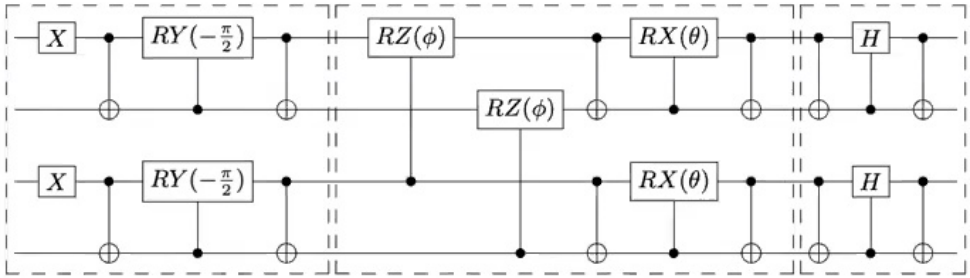

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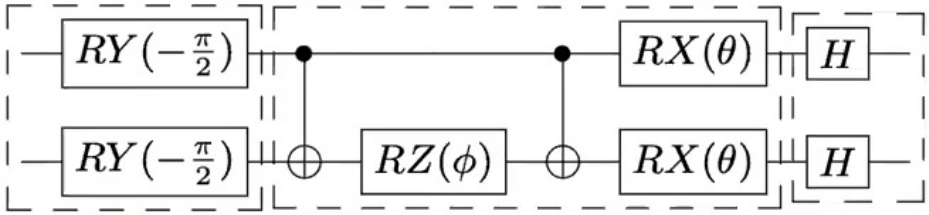

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