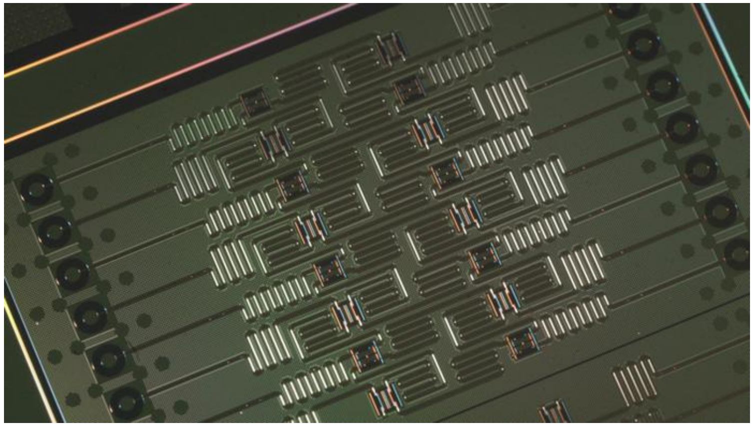
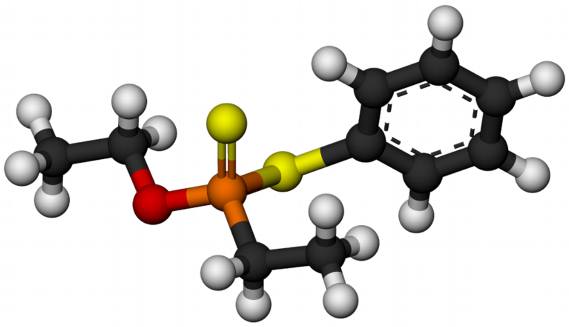
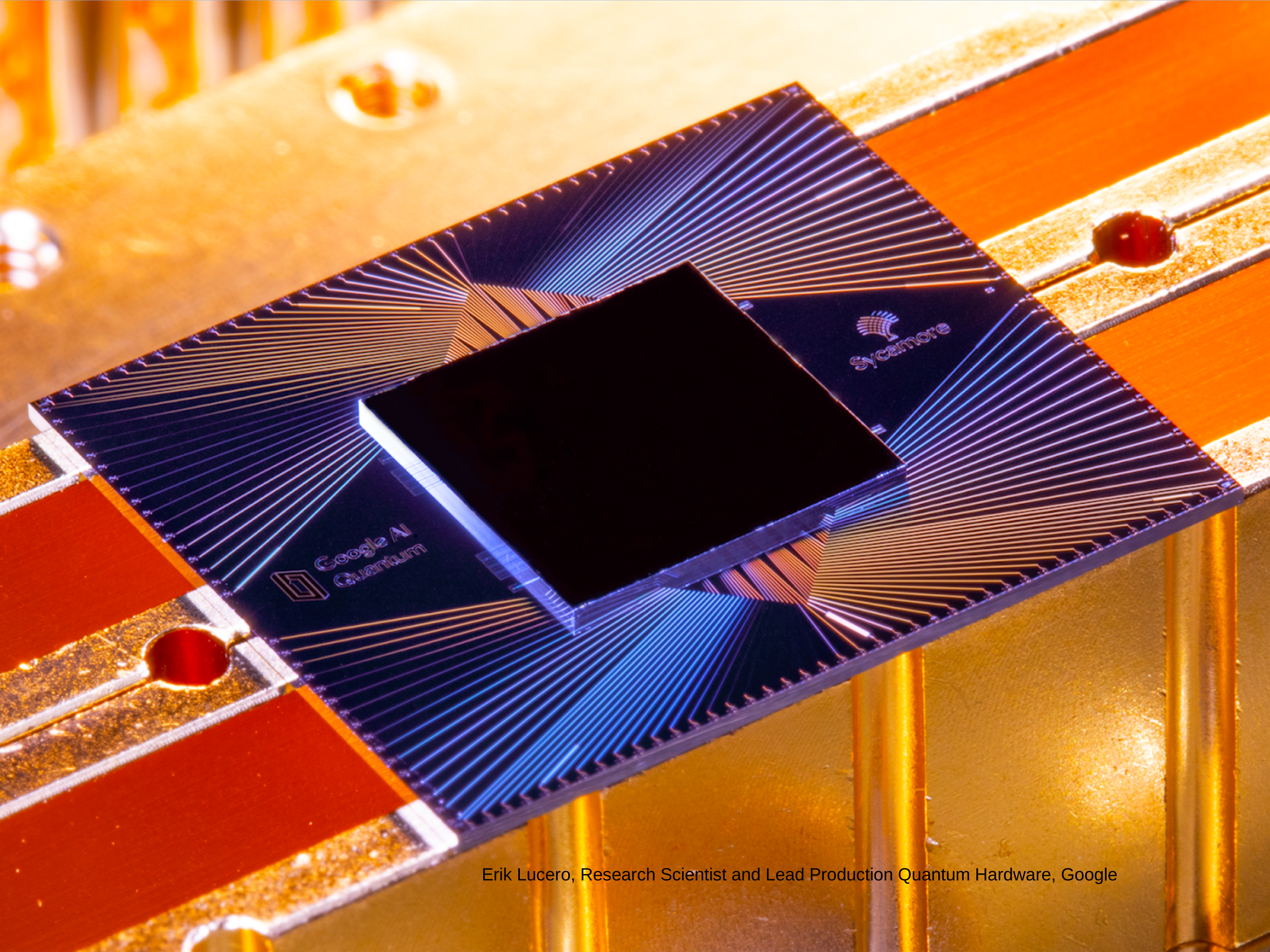
Solving quantum mechanical problems with quantum computers

Michael Marthaler
HQS Quantum Simulations, Karlsruhe







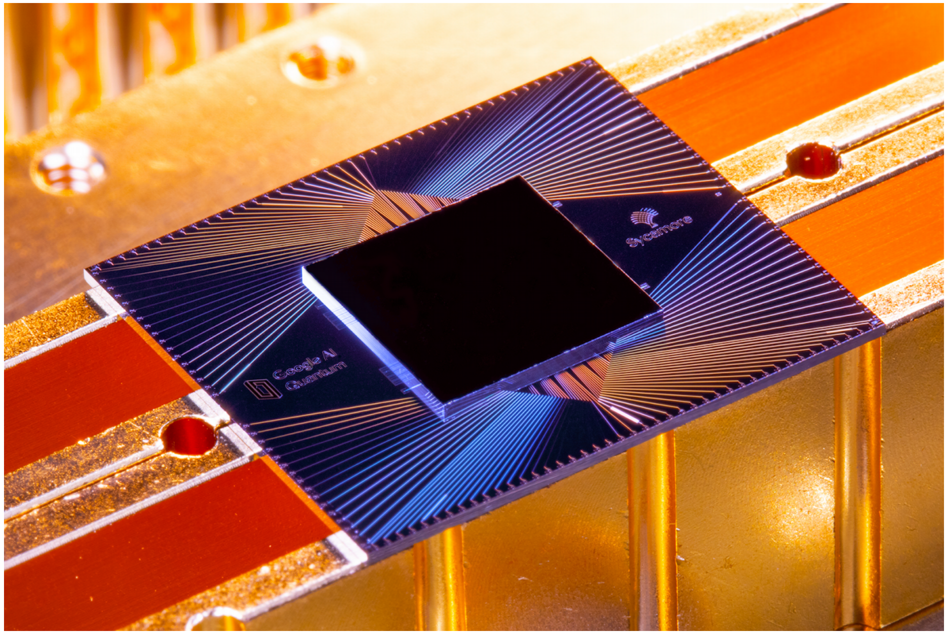
Erik Lucero, Research Scientist and Lead Production Quantum Hardware, Google

Quantum supremacy

53 Qubits:

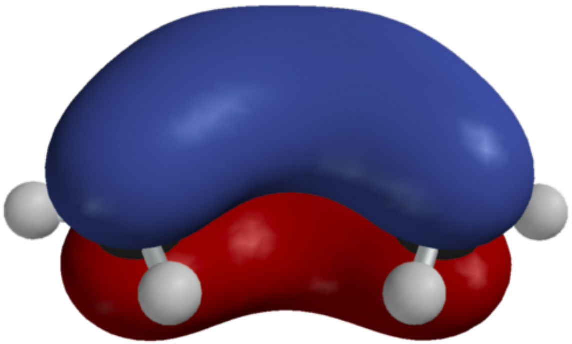
$$\begin{pmatrix} a_0 \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ \cdots \\ a_{2^{53}-1} \end{pmatrix} \xrightarrow[\text{with probability } |a_{\ldots}|^2]{\text{Measure}} |01\ldots11\rangle$$

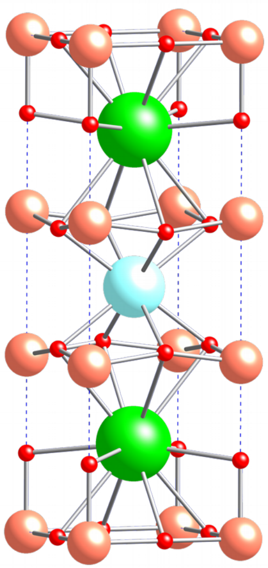
Nature **574**, 505 (2019)



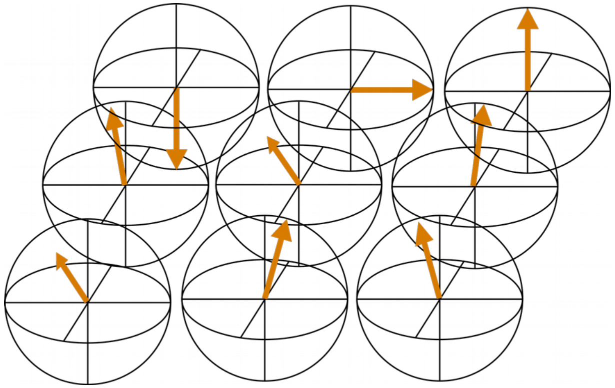
What can a quantum computer simulate?

Simulating the dynamics of a molecule or solid.



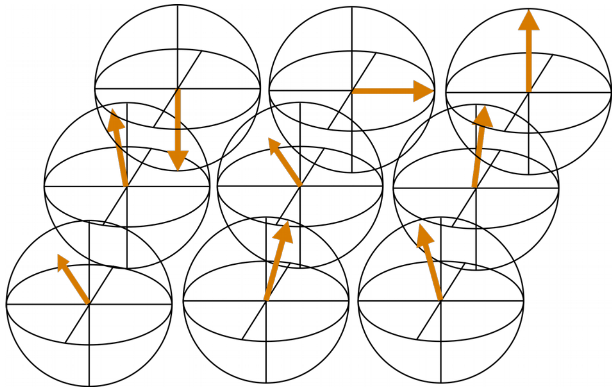


Dynamics of coupled spins.



What can a quantum computer simulate?

Dynamics of coupled spins.



Dynamics: $U(t) = e^{-iHt}$

Quantum advantage at approximately 50 Spin
→ 50 Qubits

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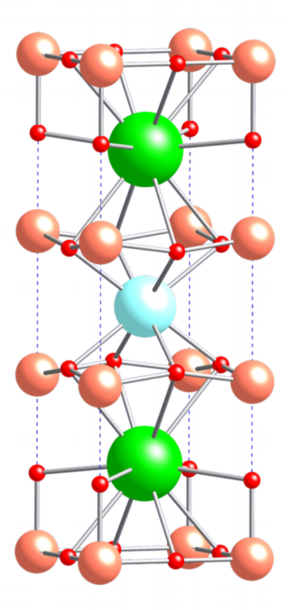
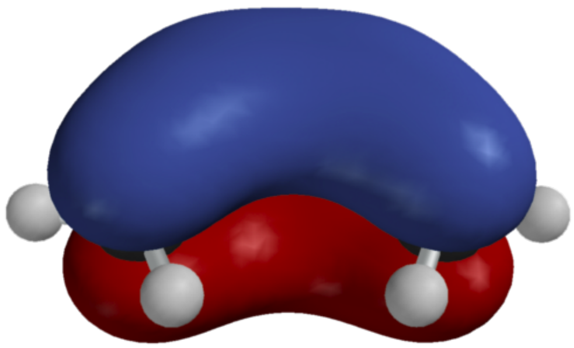
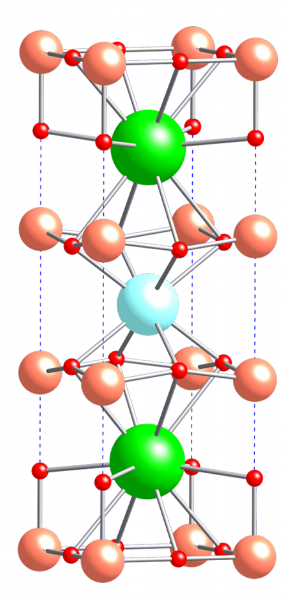


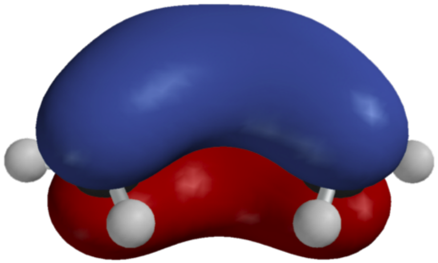
1. Simulating the time evolution under a fermionic Hamiltonian





Fermionic systems

Simulating the dynamics of a molecule or solid.



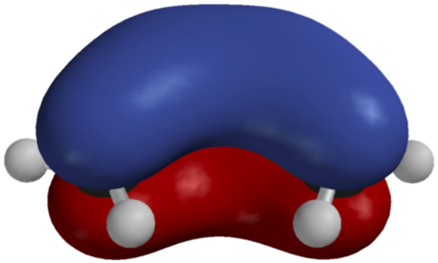
$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} v_{ijkl} c_i^\dagger c_k^\dagger c_l c_j$$

Number of terms: N^4

HQS QUANTUM SIMULATIONS

Fermionic systems: time evolution

Simulating the dynamics of a molecule or solid.



$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} v_{ijkl} c_i^\dagger c_k^\dagger c_l c_j$$

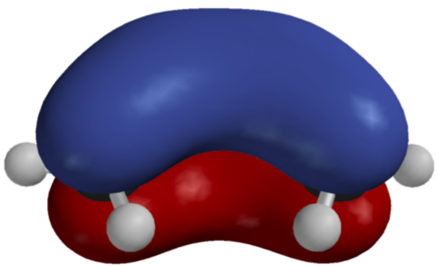
Number of terms: N^4

Time evolution: $U(t) = e^{-iHt}$

QUANTUM SIMULATIONS

Trotter expansion

Simulating the dynamics of a molecule or solid.



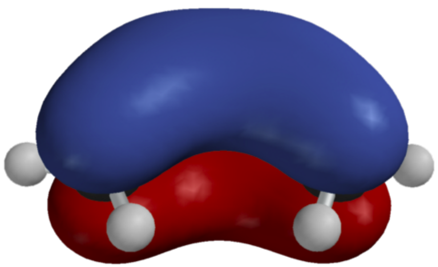
$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} v_{ijkl} c_i^\dagger c_k^\dagger c_l c_j = \sum_\xi H_\xi$$

Number of terms: N^4

Time evolution: $U(t) = e^{-iHt} = \left(e^{-iHt/n}\right)^n \approx \left(\prod_\xi e^{-iH_\xi \delta t}\right)^n$

Jordan Wigner transformation

Simulating the dynamics of a molecule or solid.



$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} v_{ijkl} c_i^\dagger c_k^\dagger c_l c_j = \sum_\xi H_\xi$$

$$H_{\xi'} = v_{ijkl}(c_i^\dagger c_k^\dagger c_l c_j + \text{h.c.})$$

$$\longrightarrow \quad e^{-iH_{\xi'}\delta t}$$

Jordan Wigner transformation: $c_i = \prod_{j<i}(-\sigma_z^j)\sigma_-^i$

$$c_i^\dagger c_k^\dagger c_l c_j + \text{h.c.} = \sigma_z^0 \sigma_z^1 \ldots \sigma_x^i \ldots \sigma_x^k \ldots + \ldots$$

Quantum computing

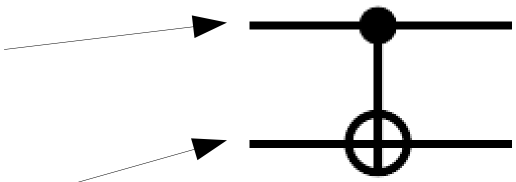
Pauli matrices and qubit states:

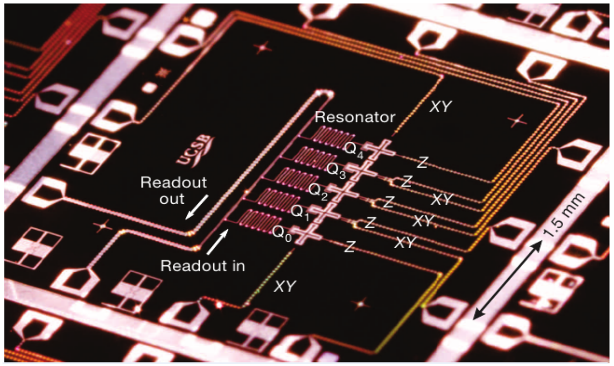
$$\sigma_\pm = \sigma_x \pm i\sigma_y \quad \sigma_+|0\rangle = |1\rangle \quad \sigma_-|1\rangle = |0\rangle \quad \sigma_z|0\rangle = -|0\rangle \quad \sigma_z|1\rangle = |1\rangle$$

Standard Depiction of qubit operations:

Time line of qubit 1

Time line of qubit 2





Nature **508**, 500 (2014)

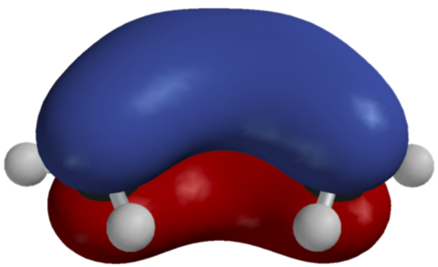
Depicted is a CNOT two qubit gate, which applies the following operation:

$$|00\rangle \rightarrow |00\rangle \quad |01\rangle \rightarrow |01\rangle$$

$$|10\rangle \rightarrow |11\rangle \quad |11\rangle \rightarrow |10\rangle$$

Implementation

Simulating the dynamics of a molecule or solid.

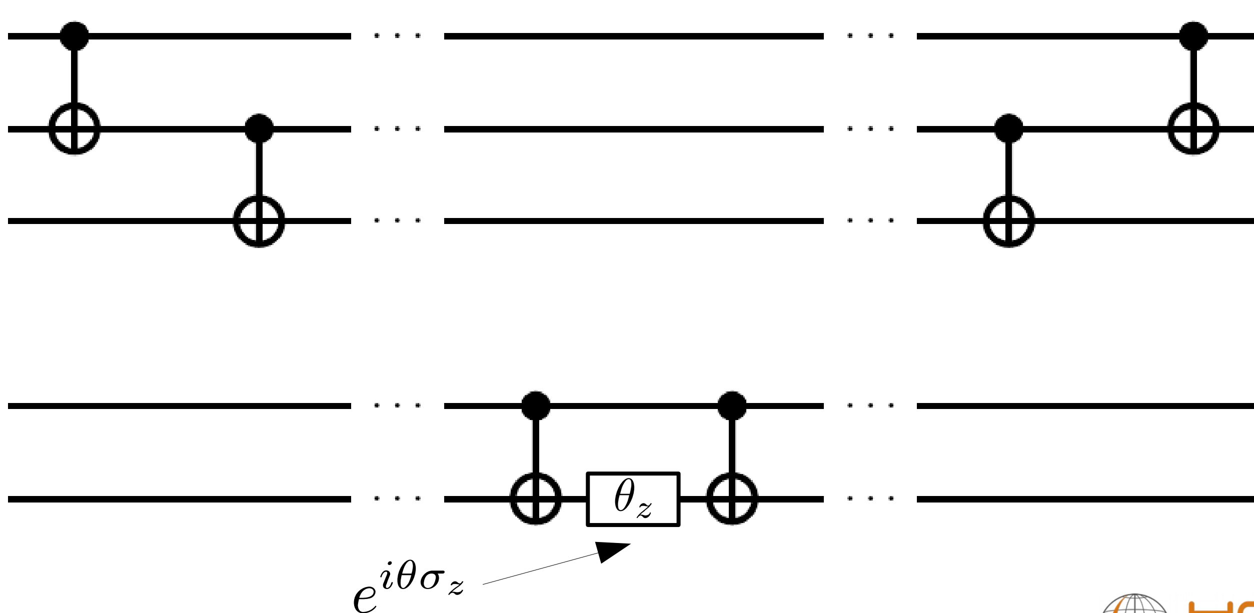


$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} v_{ijkl} c_i^\dagger c_k^\dagger c_l c_j = \sum_{\xi} H_\xi$$

$$\rightarrow \quad e^{-iH_{\xi'}\delta t}$$

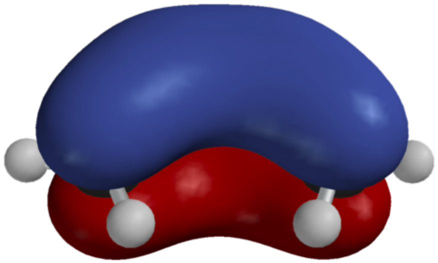
$$c_i^\dagger c_k^\dagger c_l c_j + \text{h.c.} = \sigma_z^0 \sigma_z^1 \ldots \sigma_x^i \ldots \sigma_x^k \ldots + \ldots$$

$$e^{i\theta\sigma_z^1 \ldots \sigma_z^N} =$$



Scaling

Simulating the dynamics of a molecule or solid.



$$H_S = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} v_{ijkl} c_i^\dagger c_k^\dagger c_l c_j$$
$$= \sum_\xi H_\xi$$

Number of terms: N^4

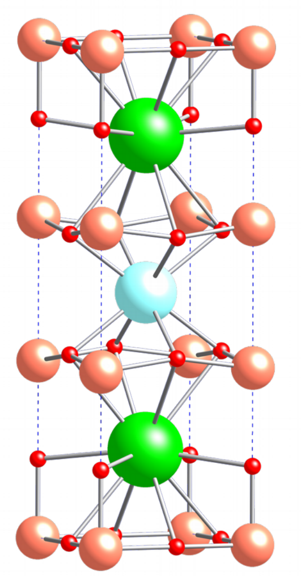
Jordan-Wigner: N

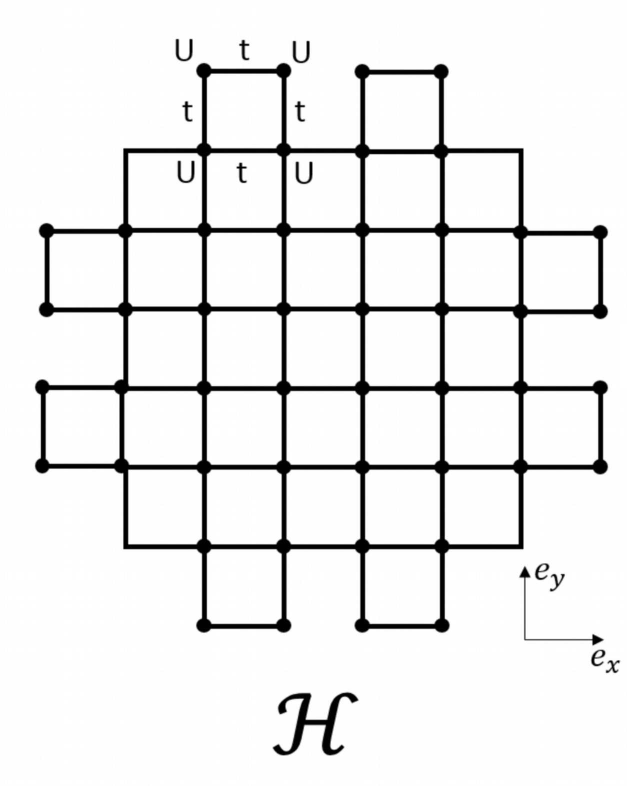
Time evolution: $U(t) = \left(\prod_\xi e^{-iH_\xi \delta t} \right)^n \quad \delta t = \frac{t}{n}$

How many Trotter-steps: $n = n(N)$

Scaling: N^5 or worse

2. Lattice Models: Simulating the time evolution



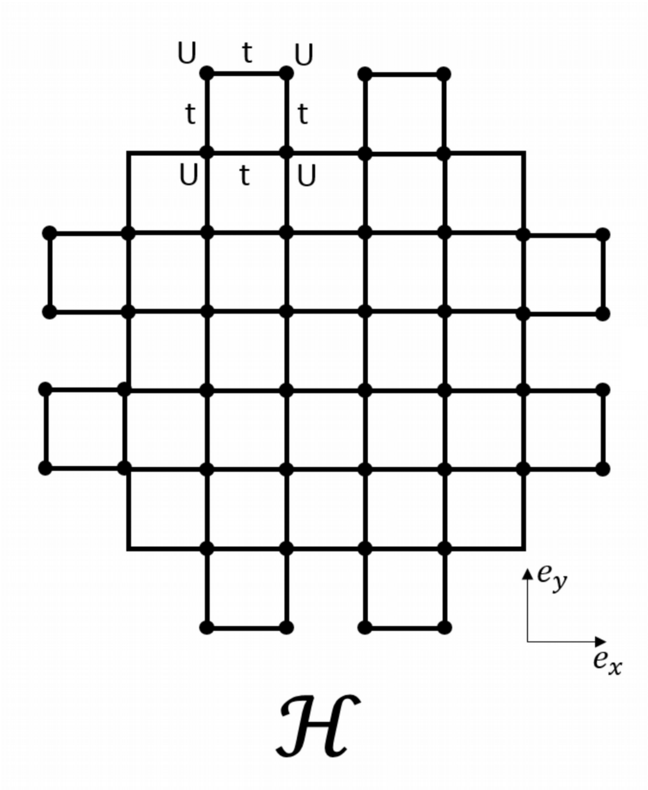


P.-L. Dallaire-Demers and F. K. Wilhelm-Mauch,
Phys. Rev. A **93**, 032303

Density-Density interaction

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ij} U_{ij} c_i^\dagger c_i c_j^\dagger c_j = \sum_{ij} H_{ij}$$

$$U(t) = \left(\prod_{ij} e^{-iH_{ij}\delta t} \right)^n \quad \delta t = \frac{t}{n}$$



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Quantum computing

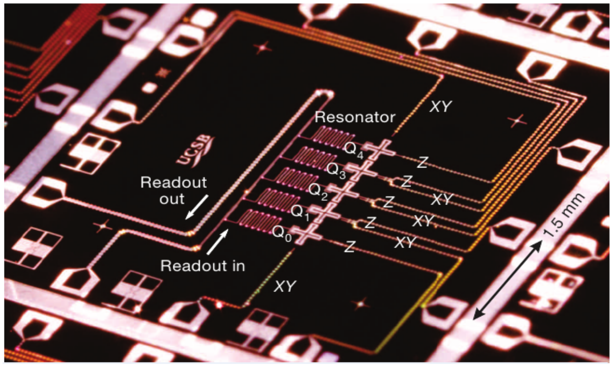
SWAP Operation:

$$|ab\rangle \rightarrow |ba\rangle$$

fSWAP Operation:

$$|ab\rangle \rightarrow (-1)^{a\,b}|ba\rangle$$

$$\mathrm{fSWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$



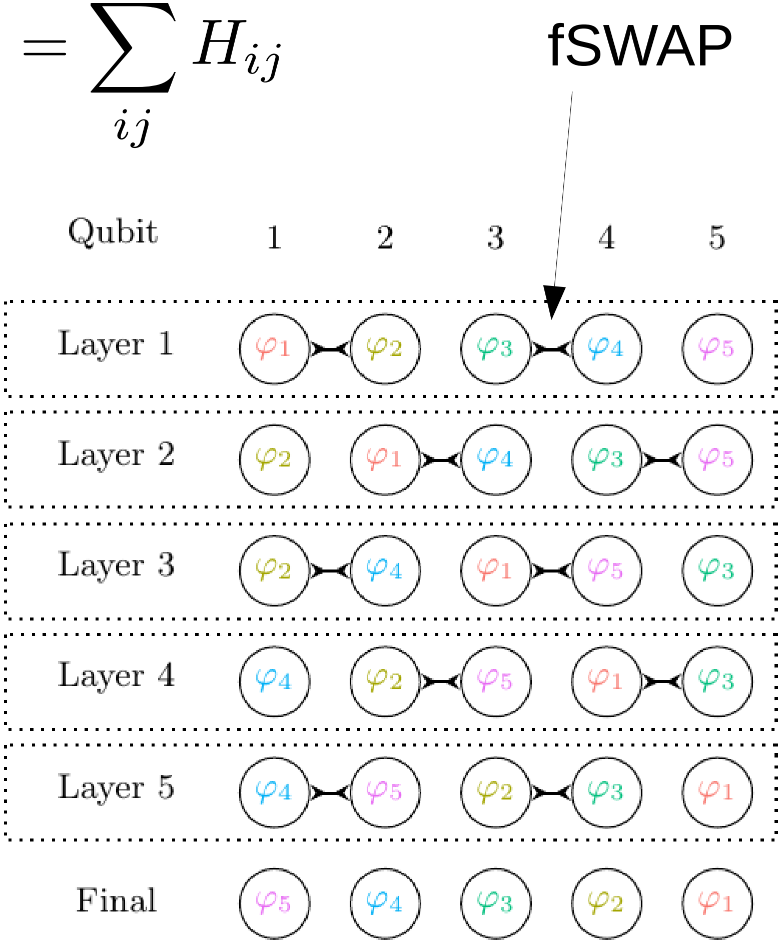
Nature **508**, 500 (2014)

Fermionic swap networks

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ij} U_{ij} c_i^\dagger c_i c_j^\dagger c_j = \sum_{ij} H_{ij}$$

$$U(t) = \left(\prod_{ij} e^{-iH_{ij}\delta t} \right)^n \qquad \delta t = \frac{t}{n}$$

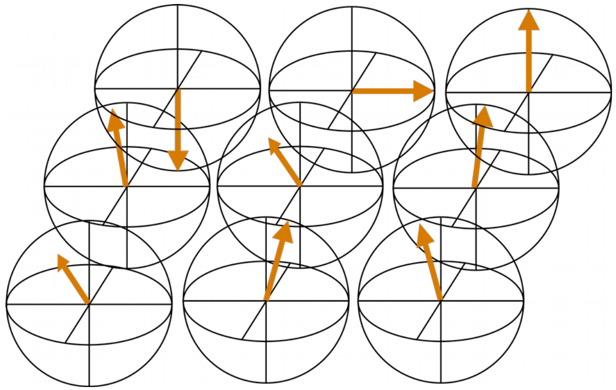
Gate-depth per Trotter-step: N



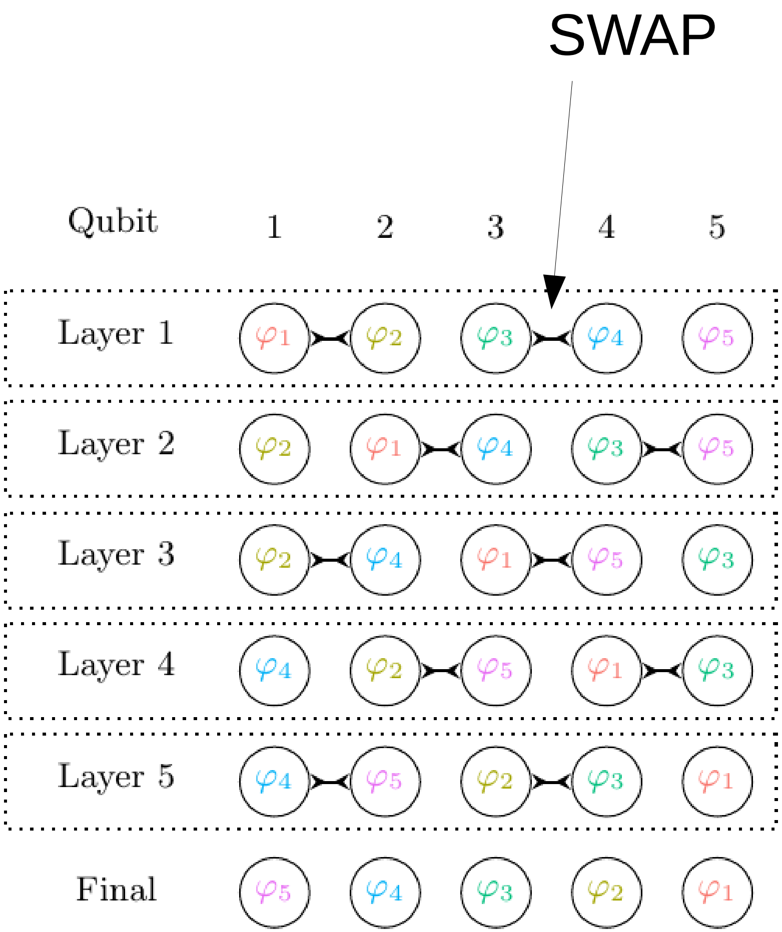
I, D. Kivlichan, J. McClean, N. Wiebe, C. Gidney, A. Aspuru-Guzik, G. Kin-Lic Chan and R. Babbush, Phys. Rev. Lett. **120**, 110501 (2018)

Swap networks

System of coupled spins:



Gate-depth per Trotter-step: N



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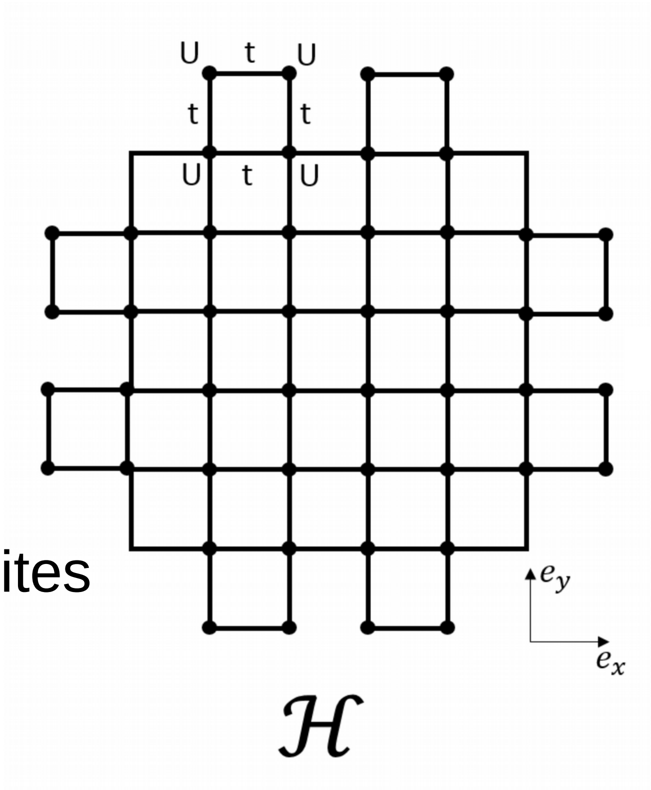
Density-Density interaction: Scaling

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ij} U_{ij} c_i^\dagger c_i c_j^\dagger c_j = \sum_{ij} H_{ij}$$

$$U(t) = \left(\prod_{ij} e^{-iH_{ij}\delta t} \right)^n \quad \delta t = \frac{t}{n}$$

Gate depth: N Gates total: N^2



Quantum advantage at approximately 50 sites
→ 100 Qubits

For half-filling!

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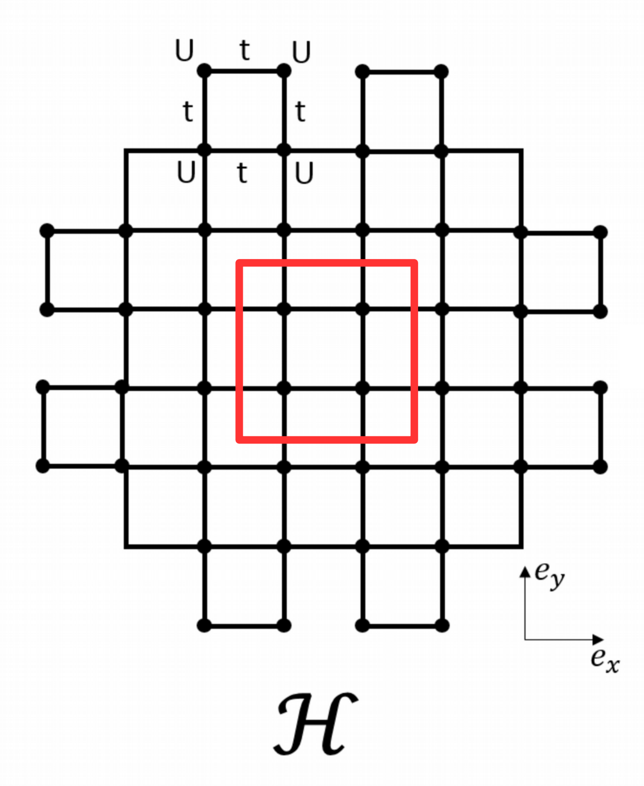
3. Lattice models: Embedding



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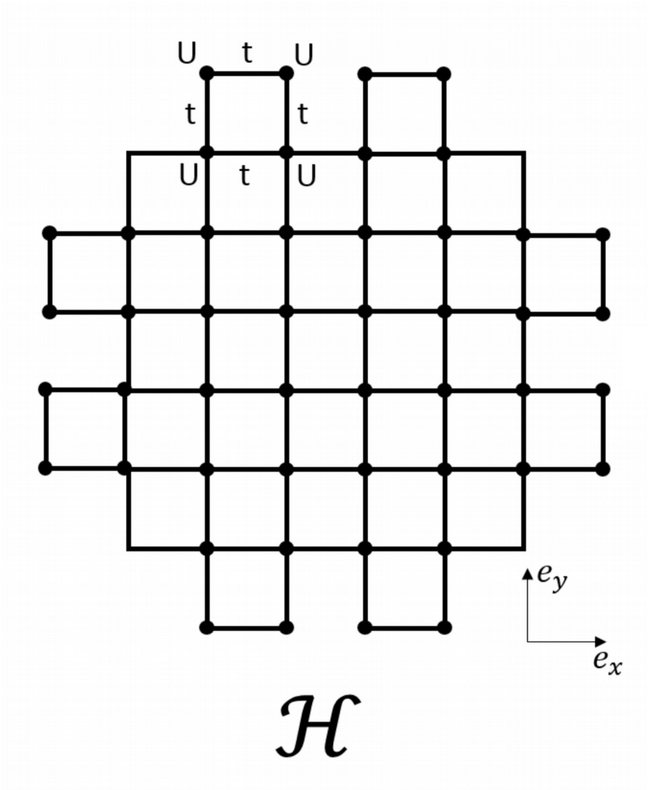
From infinite to finite

System is periodic and infinite

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ij} U_{ij} c_i^\dagger c_i c_j^\dagger c_j$$

We have to calculate properties from smaller section.

Only well established for ground state or equilibrium properties.



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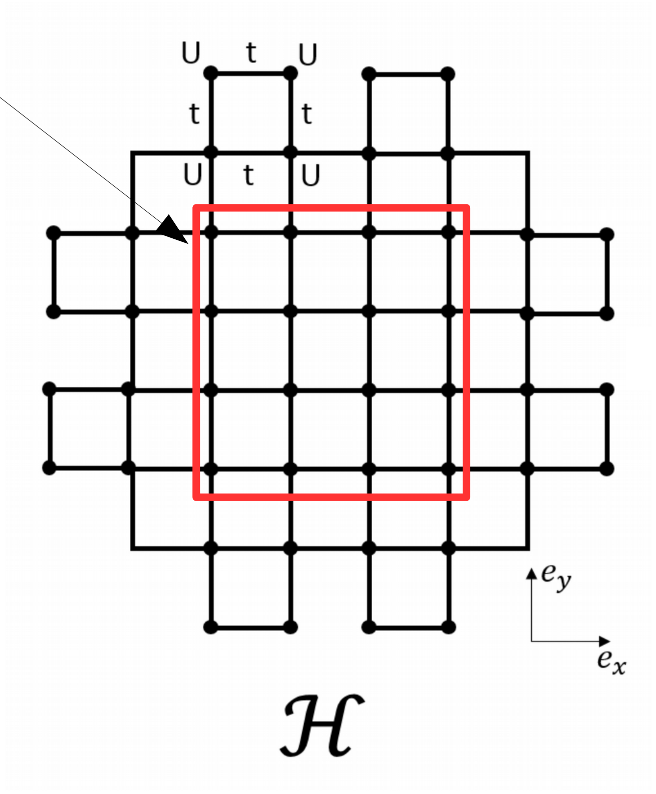
CPT: Cluster perturbation theory

Calculate cluster Green's functions $\mathbf{G}_C(\omega)$

Connect to the rest of the system as if it is non-interacting:

$$\mathbf{G}_{\text{full}}(\omega) = \frac{1}{[\mathbf{G}(\omega)]^{-1} - \mathbf{t}}$$

$\mathbf{G}_C(\omega)$ can in principle be calculated on a quantum computer



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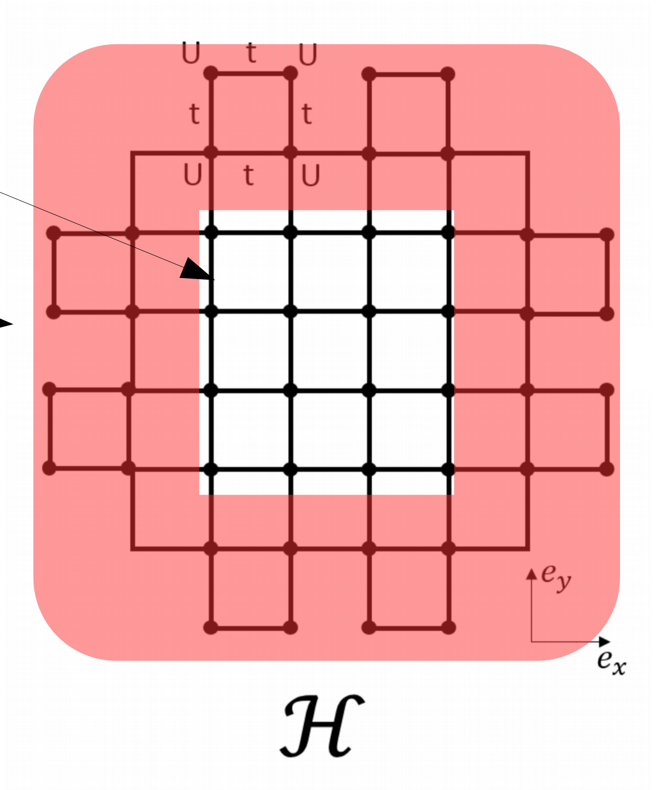
DMFT: Dynamical mean field theory

Fully interacting cluster

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ij} U_{ij} c_i^\dagger c_i c_j^\dagger c_j$$

Non-interacting bath

The bath is adjusted in a self-consistent way.



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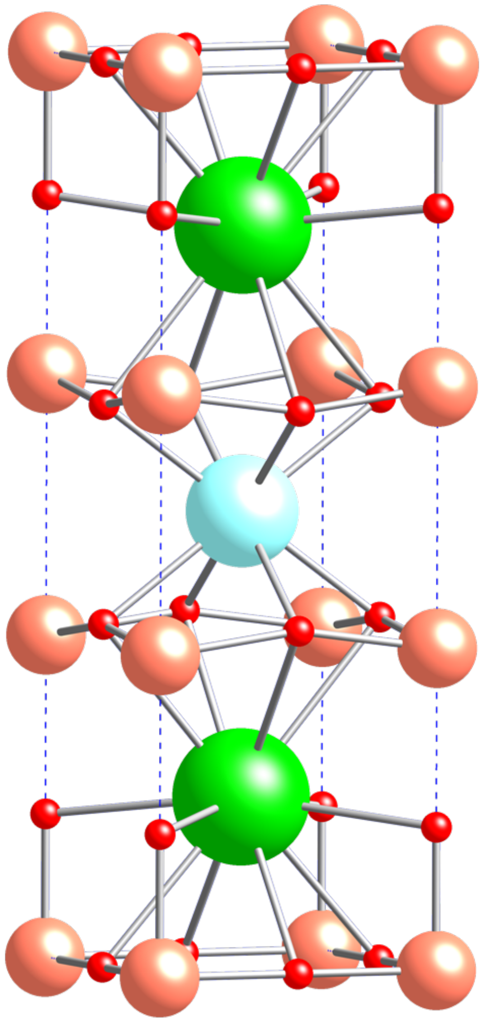
4. Finding the ground state



Variational Hamiltonian Ansatz

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ij} U_{ij} c_i^\dagger c_i c_j^\dagger c_j$$

$$\mathrm{h}_1 = \sum_{ij} t_{ij} c_i^\dagger c_j \ , \ h_2 = \sum_{ij} U_{ij} c_i^\dagger c_i c_j^\dagger c_j$$

$$U_1^s = e^{i\theta_1^s h_1 t} \qquad U_2^s = e^{i\theta_2^s h_2}$$

Step 1:

- prepare state $|1\rangle = U_1^1 U_2^1 U_2^1 U_1^1 |0\rangle$

- Measure average energy $E = \langle 1|H|1\rangle$

- find angles which minimize the average energy

Step 2:

- prepare state $|2\rangle = U_1^2 U_2^2 U_2^2 U_1^2 |1\rangle$
- etc.

Variational Hamiltonian Ansatz

$$\mathrm{h}_1 = \sum_{ij} t_{ij} c_i^\dagger c_j \,,\; h_2 = \sum_{ij} U_{ij} c_i^\dagger c_i c_j^\dagger c_j$$

$$U_1^s = e^{i\theta_1^s h_1 t} \qquad U_2^s = e^{i\theta_2^s h_2}$$

Step s:

- prepare state $|s\rangle = U_1^s U_2^s U_2^s U_1^s |s-1\rangle$

- Measure average energy $E = \langle s|H|s\rangle$

- find angles which minimize the average energy

Choose number of VHA Steps s

Optimize step by step or all at once.

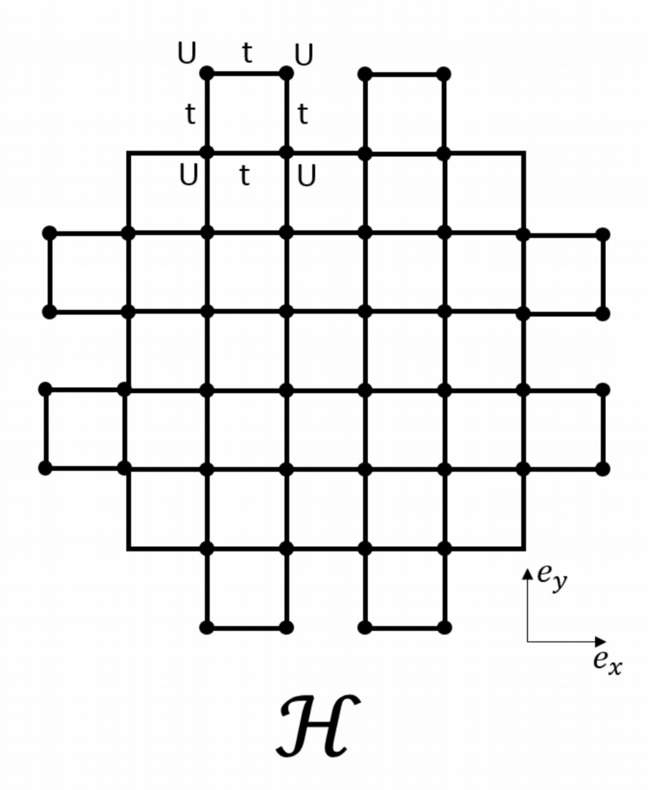
Trotterization

Implementation of the unitary operator:

$$\mathrm{h}_2 = \sum_{ij} U_{ij} c_i^\dagger c_i c_j^\dagger c_j = \sum_{ij} h_{ij}$$

Trotterization

$$U_2^s = e^{i\theta_2^s h_2} = e^{i\theta_2^s \sum_{ij} h_{ij}} \approx \left(\prod_{ij}^{N} e^{i\theta_2^s h_{ij}/n} \right)^n$$



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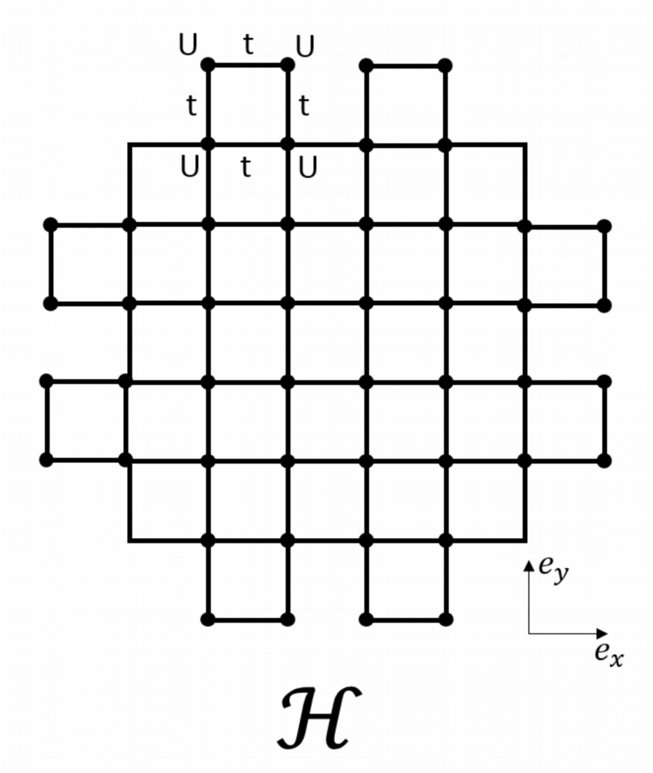
Hubbard Model with errors

Gates with errors, e.g.:

$$e^{-i\frac{U}{4}\sigma_i^z\sigma_{i+N}^z} \longrightarrow e^{-i\left(\frac{U}{4}+\delta\phi\right)\sigma_i^z\sigma_{i+N}^z}$$

Random over-rotation.
Considered to be constant
in the following.

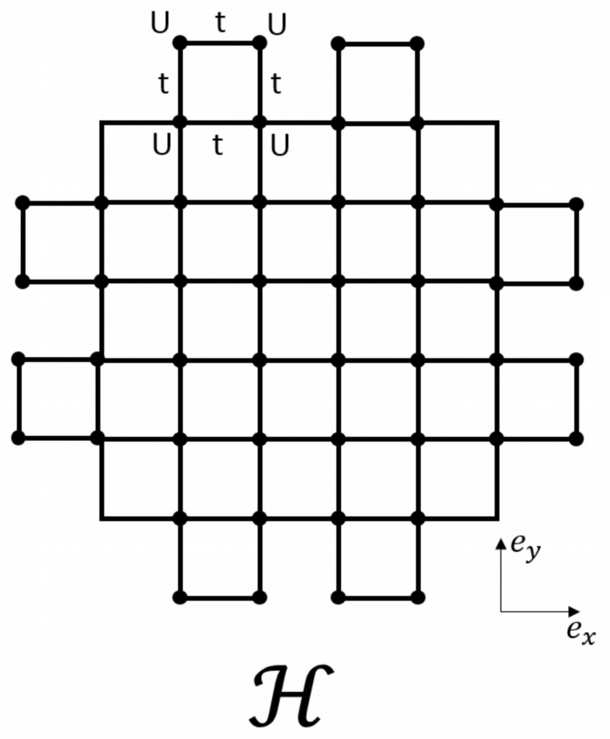


Hubbard Model with errors: ground state fidelity

VHA, 3 x 3 Hubbard Model:

$\mathcal{F}$		100.00	99.999	99.990	99.900	99.500
S	4	99.1	98.97	98.23	95.6	86.24
	6	99.59	99.46	99.27	95.55	90.06
	8	99.93	99.74	99.01	97.35	90.14
	10	99.97	99.89	99.77	98.04	90.69

Achievable ground state fidelity with errors.



J.-M. Reiner, F. Wilhelm-Mauch, G. Schön, M. Marthaler, Quantum Sci. Technol. 4, 035005 (2019)

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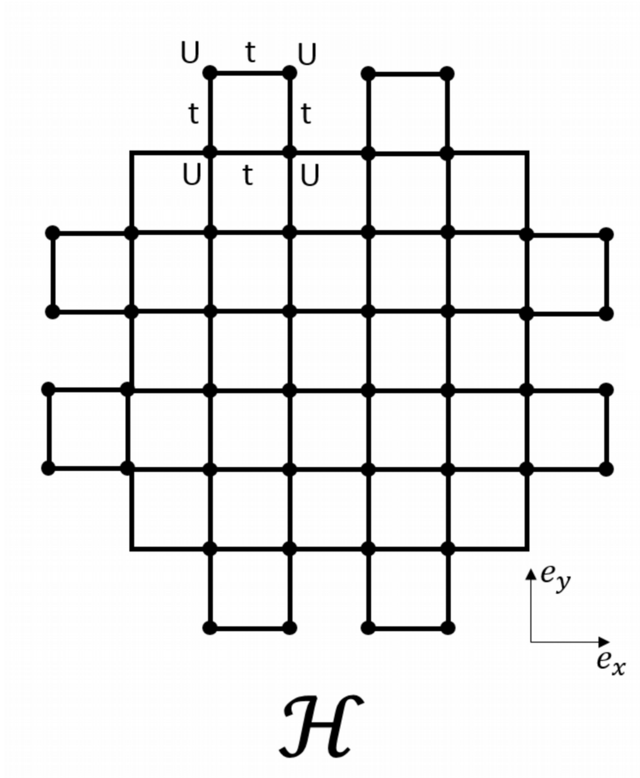
Effect of variational approach

VHA, 2 x 2 Hubbard Model:

$\mathcal{F}$		**99.90**	**99.90***
s	**2**	99.24	94.44
	3	99.56	93.54
	4	99.68	88.77
	5	99.82	83.69



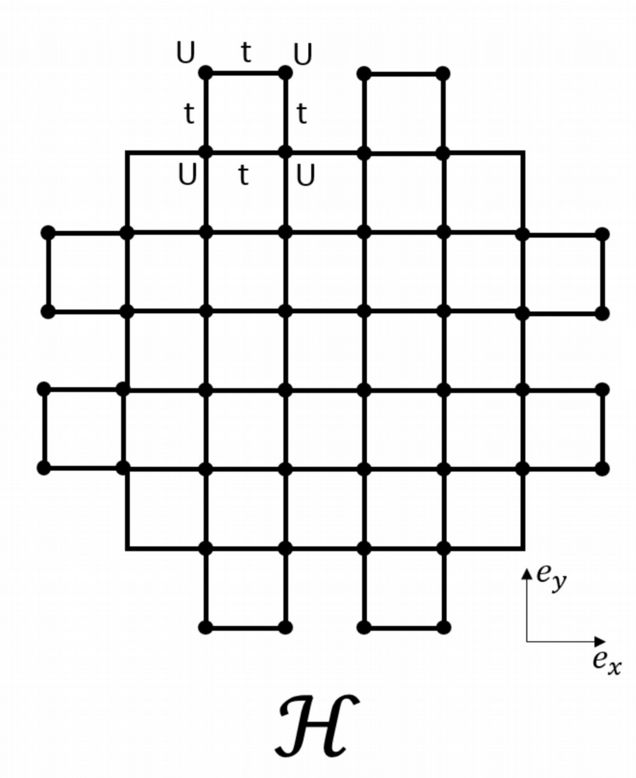
Variational algorithms improve ground state fidelity.

J.-M. Reiner, F. Wilhelm-Mauch, G. Schön, M. Marthaler, Quantum Sci. Technol. 4, 035005 (2019)

Improved initial guess

VHA, 3 x 3 Hubbard Model:

	$\mathcal{F}$	**100.00**	**99.90**	**99.90**
S	**4**	99.1	95.6	Improved initial guess:
	6	99.59	95.55	
	8	99.93	97.35	
	10	99.97	98.04 →	98.91



Choice of initial guess can effect results substantially.

J.-M. Reiner, F. Wilhelm-Mauch, G. Schön, M. Marthaler, Quantum Sci. Technol. 4, 035005 (2019)

Conclusion

Simulating fully fermionic lattice models seams possible:

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ij} U_{ij} c_i^\dagger c_i c_j^\dagger c_j$$

Quantum advantage achievable with 100 qubits for models with approx. half filling.

Very difficult to simulate bosonic modes.