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Materials science and chemistry with quantum algorithms:

from the textbook to the processor

TERATEC TQCI - Quantum algorithms in the NISQ era

Thursday, November 14th 2024

Thomas Ayral
Eviden Quantum Lab, France

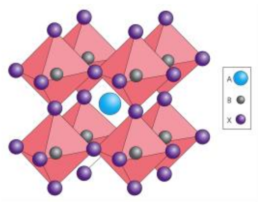
an atos business

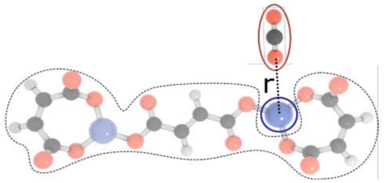
The textbook:

On the one hand:

A complex quantum system

$$i\hbar \frac{d|\Psi\rangle}{dt} = H(t)|\Psi\rangle$$





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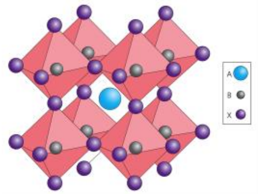
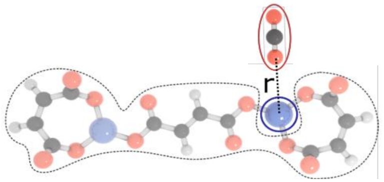
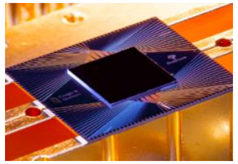


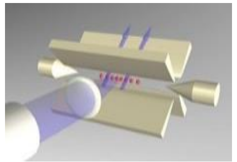


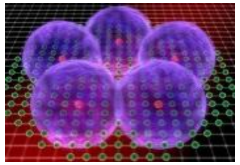
On the other hand:

A complex... artificial... quantum system

$$i\hbar \frac{d|\widetilde{\Psi}\rangle}{dt} = \widetilde{H}(t)|\widetilde{\Psi}\rangle$$







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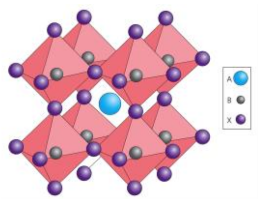

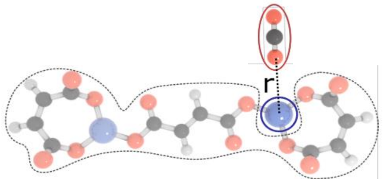

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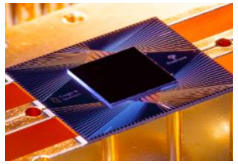

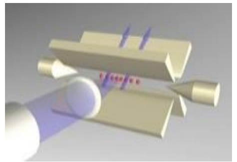

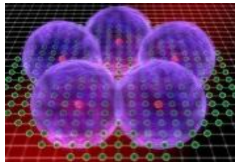

If $\widetilde{H} \approx H$, we learn something about $|\Psi\rangle$ by measuring $|\widetilde{\Psi}\rangle$!

Exponential advantage for quantum dynamics (Lloyd '96)

Materials science and chemistry: low-energy states

Ground state search:

$$H|\Psi\rangle = E|\Psi\rangle$$

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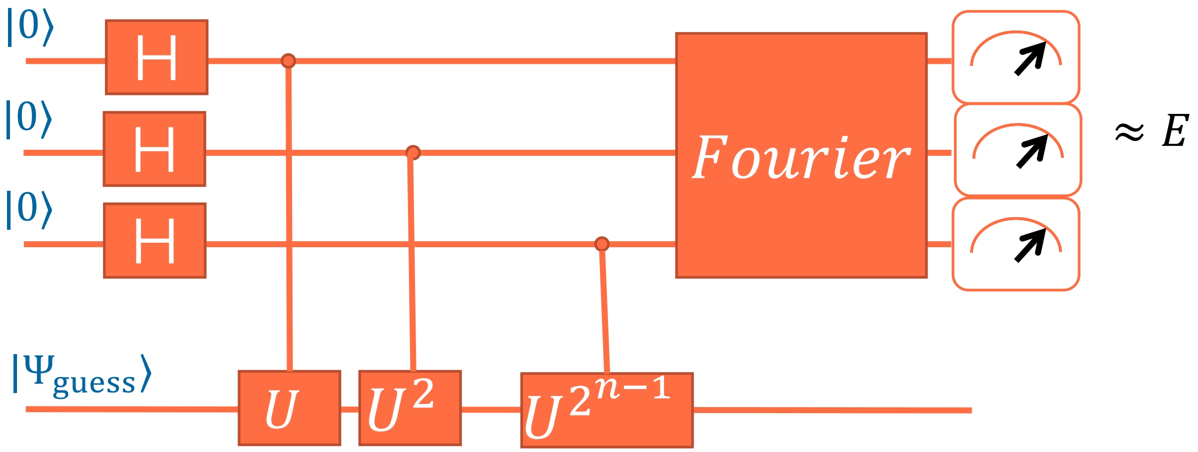
Quantum phase estimation (QPE) algorithm (Kitaev 95)



with $U = e^{-iHt/\hbar}$

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Too long!

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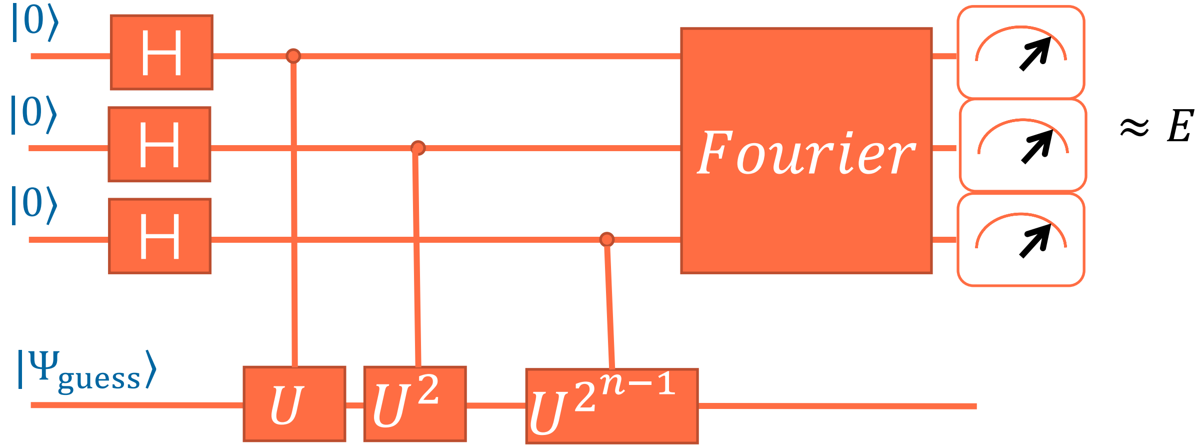

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Large Scale Quantum: Tomorrow

Quantum error corrected computers

A lot (millions) of high-quality qubits

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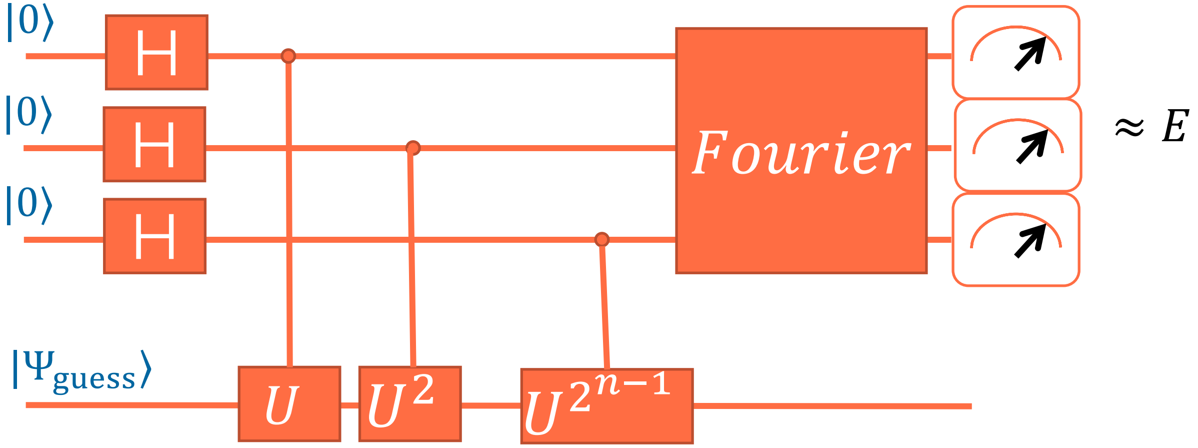

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Most advanced experiments (Rydberg, ions, superconducting qubits):

Only 10-100 physical qubits, just below threshold

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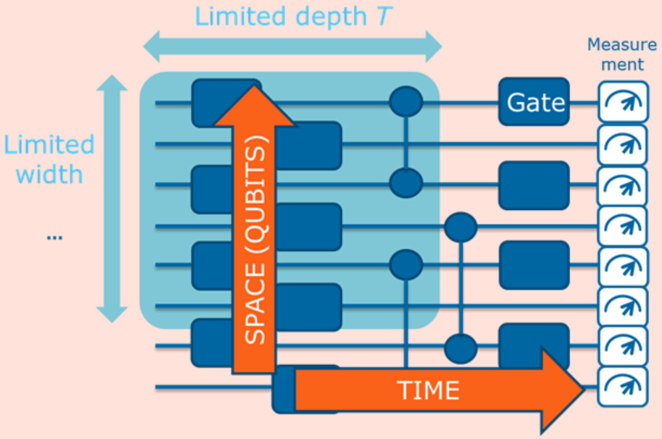
Materials science and chemistry: low-energy states

Noisy Intermediate Scale Quantum: Today

- Small number of qubits (10-1000 today)
- High error rates (100-1000 gates)



Exponential decay of fidelity:

$$F = e^{-pN_g}$$

Error per gate

Number of gates

Large Scale Quantum: Tomorrow

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Too long... also without noise?

Louvet, TA, Waintal, 2306.02620

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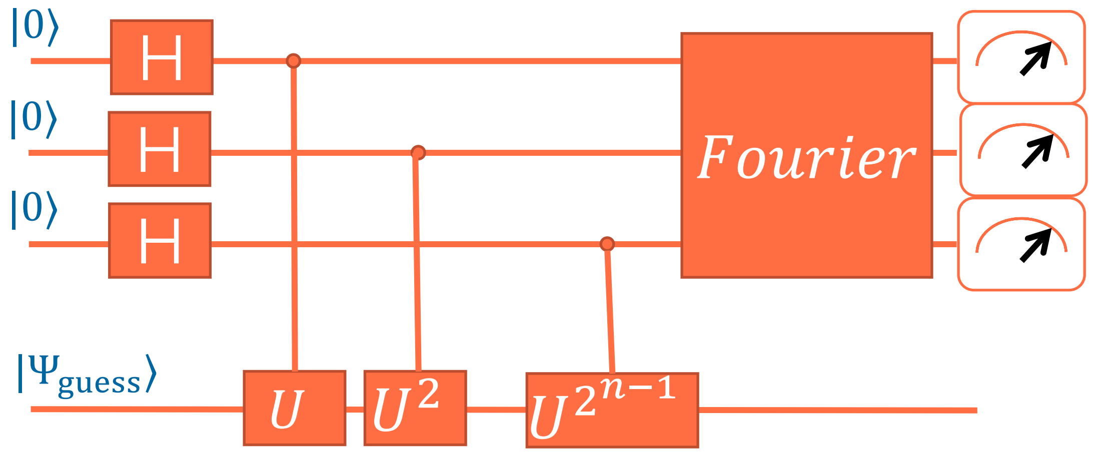

Key point: role of overlap

$$\Omega = \left|\langle\Psi_{\text{guess}}|\Psi_0\rangle\right|^2$$

Need $O(\frac{1}{\Omega})$ repetitions of QPE!

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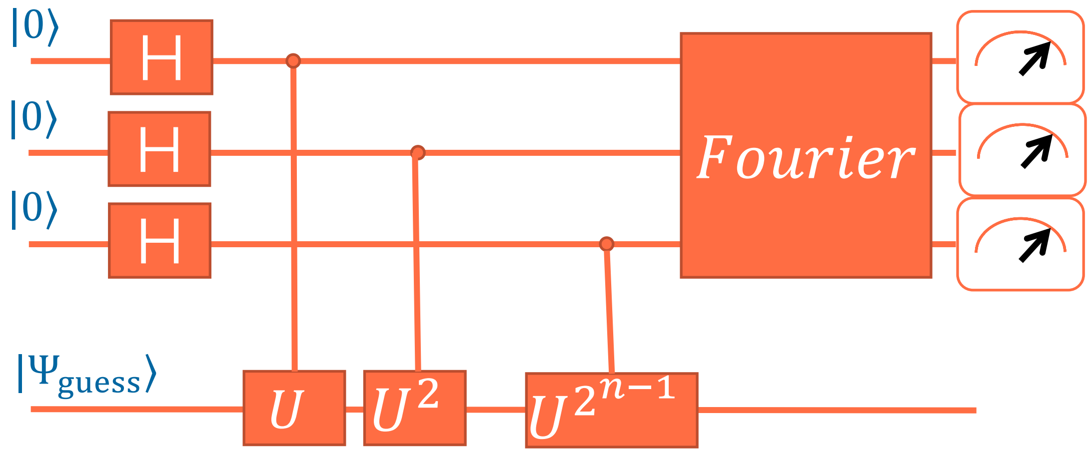

Key point: role of overlap

$$\Omega = |\langle\Psi_{\text{guess}}|\Psi_0\rangle|^2$$

Need $O(\frac{1}{\Omega})$ repetitions of QPE!

We found a formula to assess Ω given the energy + variance of Ψ_{guess} (+ estimate of E_0).

Applied it to advanced classical methods.

Outcome:
Ω decreases exponentially with molecule size!

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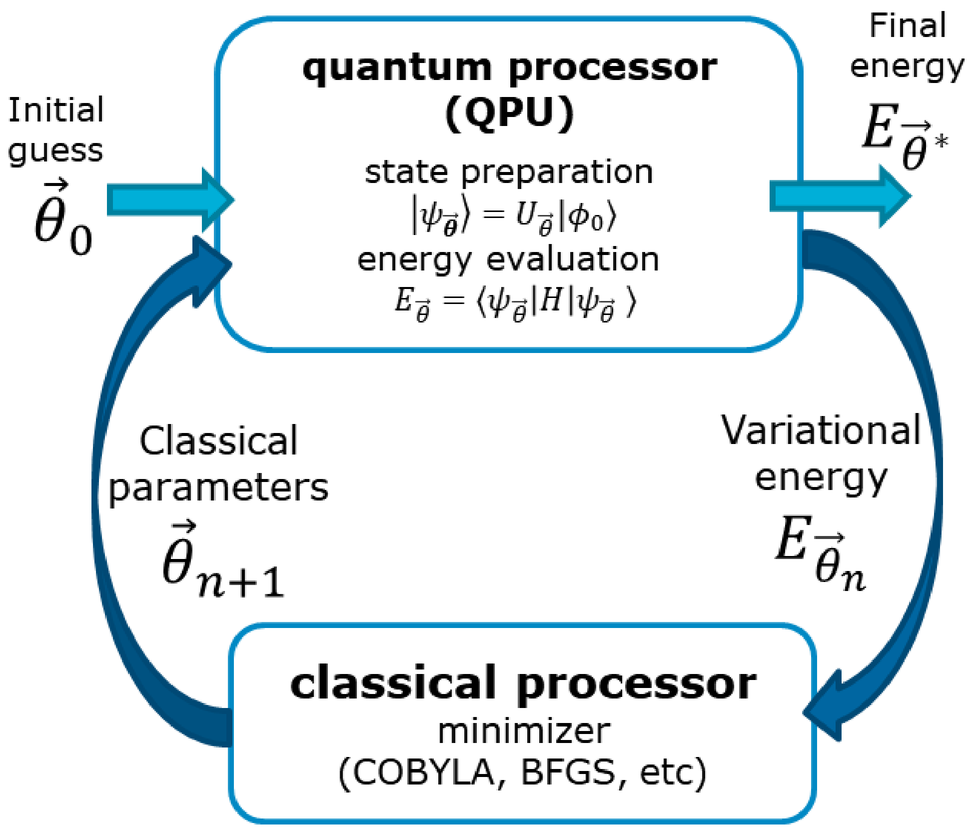
Too long!

What can one do with today's processors?

The bread-and-butter NISQ algorithm: the variational quantum eigensolver

(Peruzzo et al 2014)



The bread-and-butter NISQ algorithm: the variational quantum eigensolver

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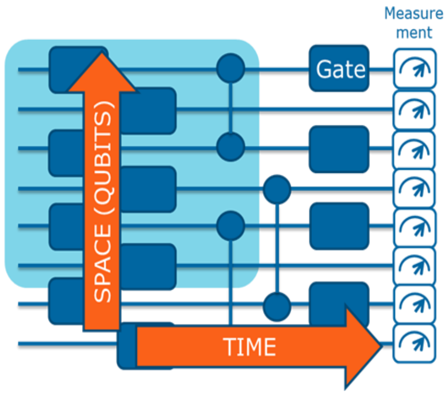
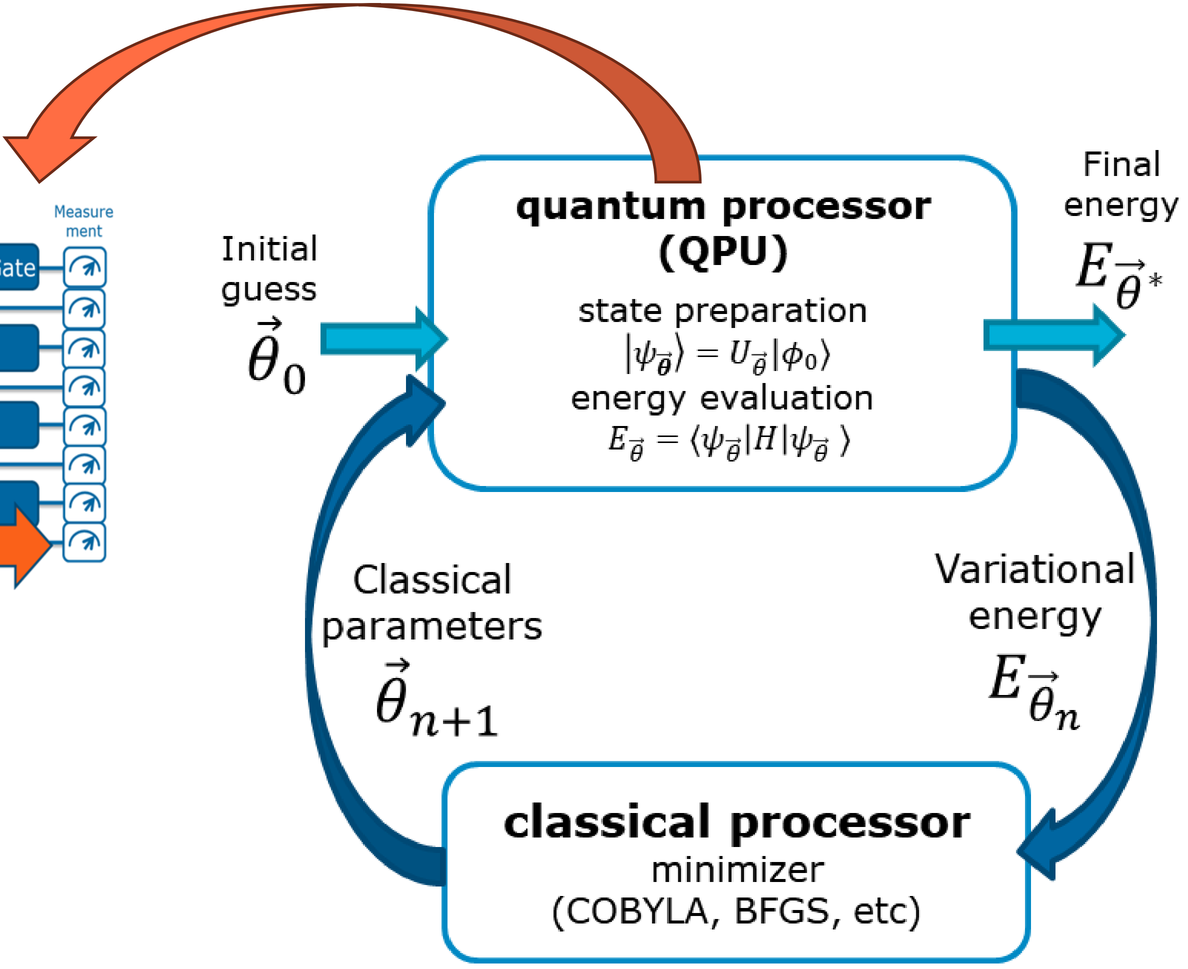
Parametric circuit $U_{\vec{\theta}}$:

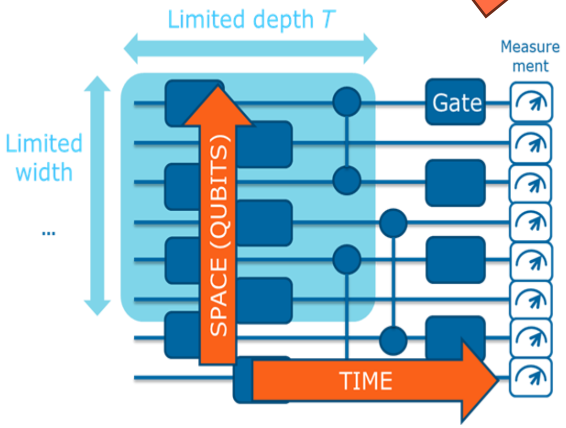




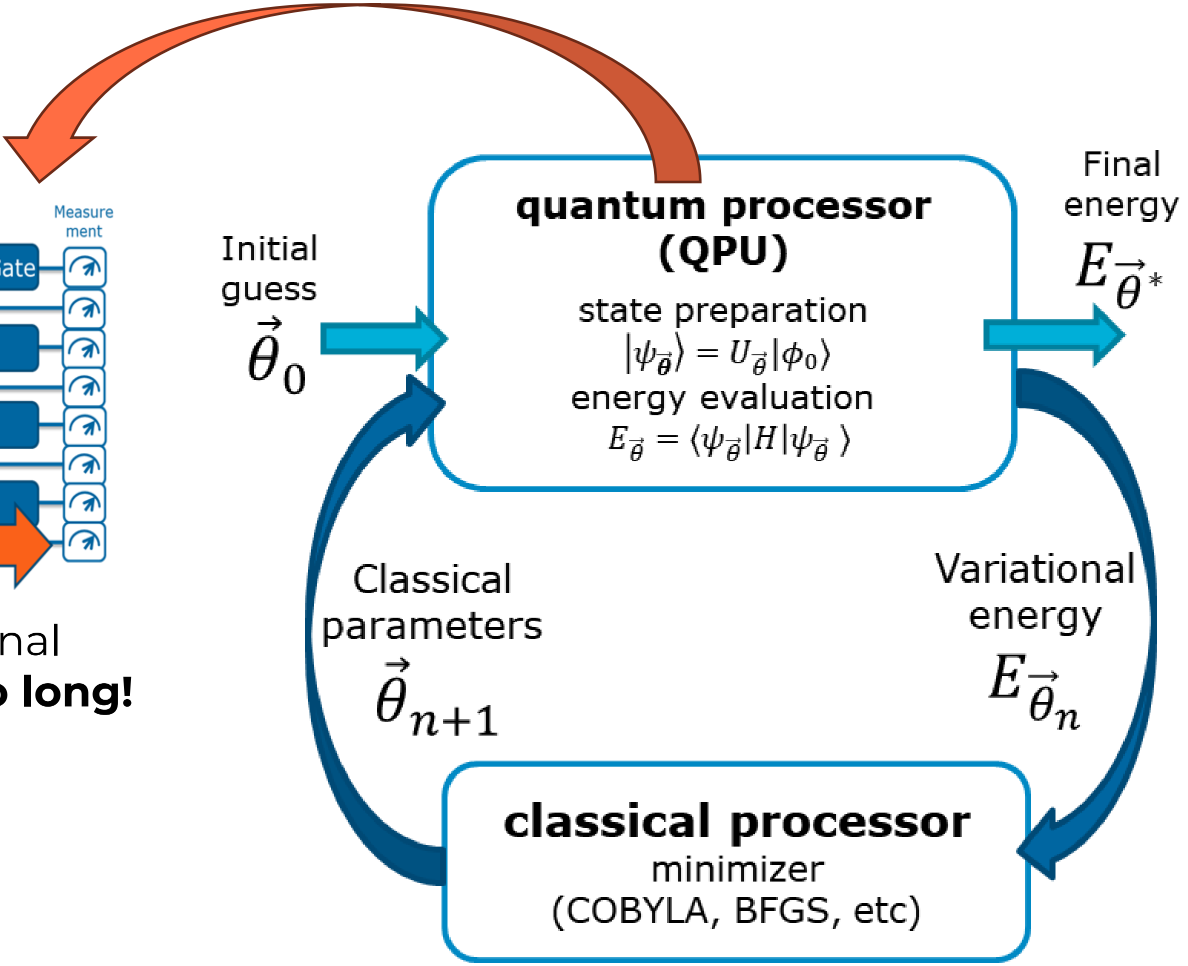
Idea: try to minimize use of quantum resources

Known issues with the variational quantum eigensolver

Parametric circuit $U_{\vec{\theta}}$:



Interesting variational circuits **are still too long!**



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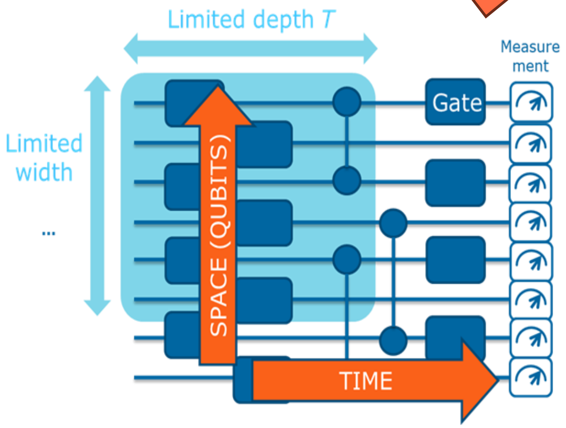

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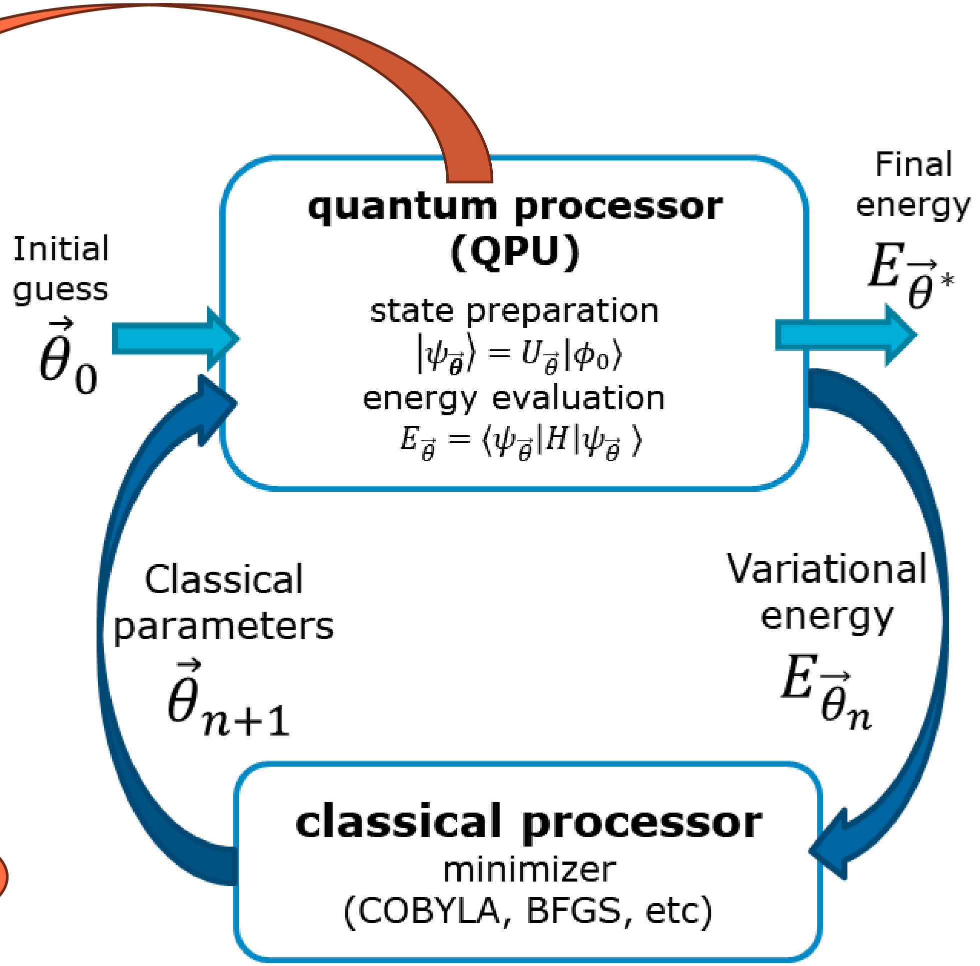
$$F = e^{-pN_g}$$

Error per gate

Number of gates



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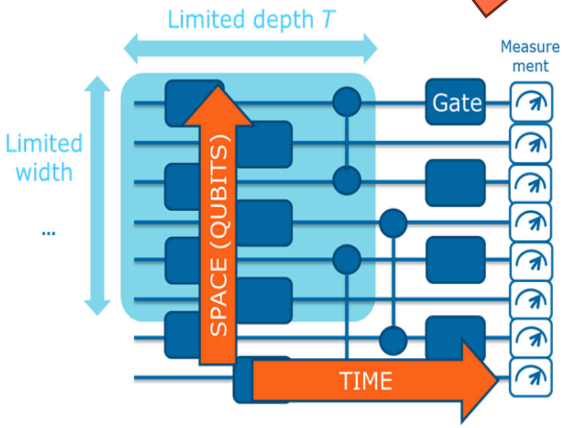

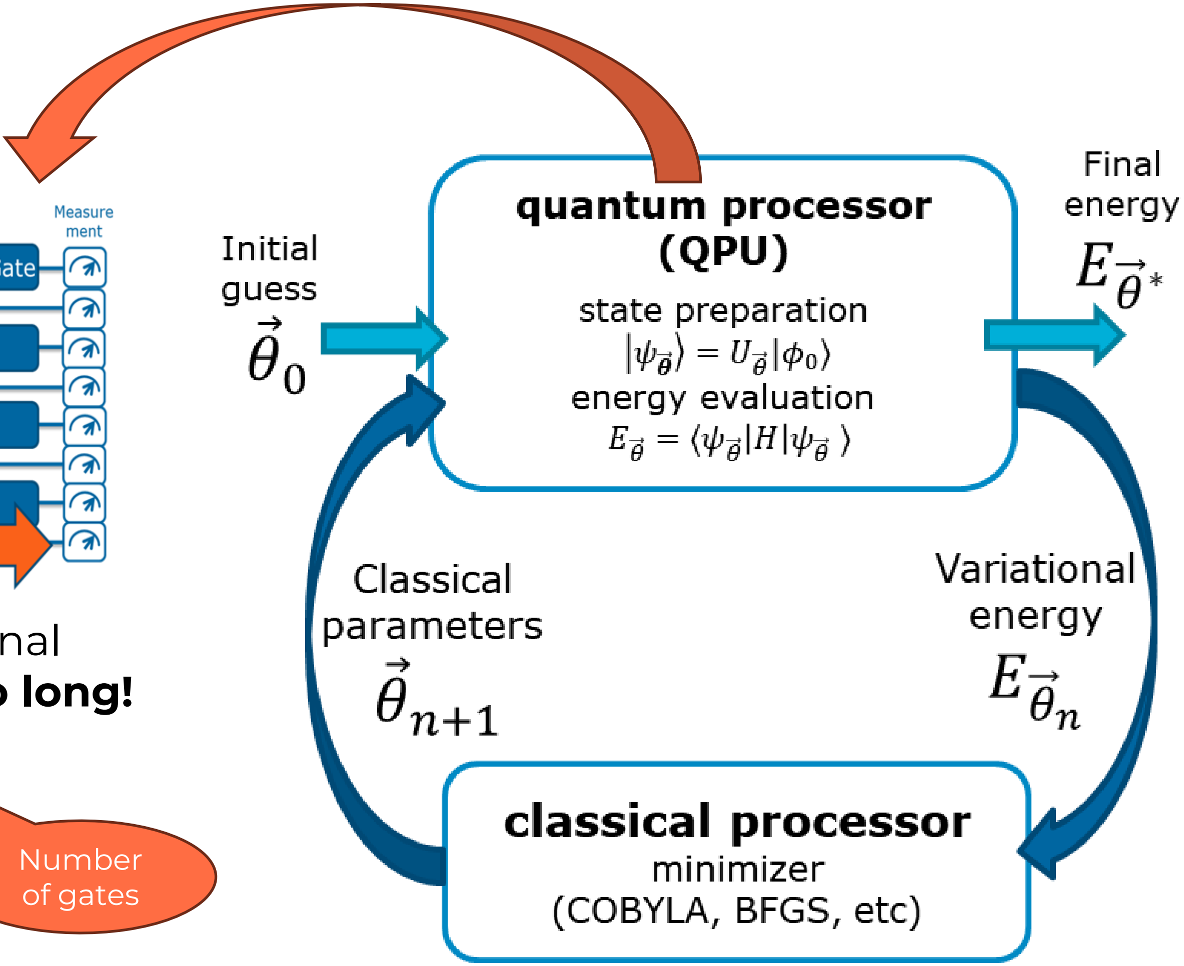

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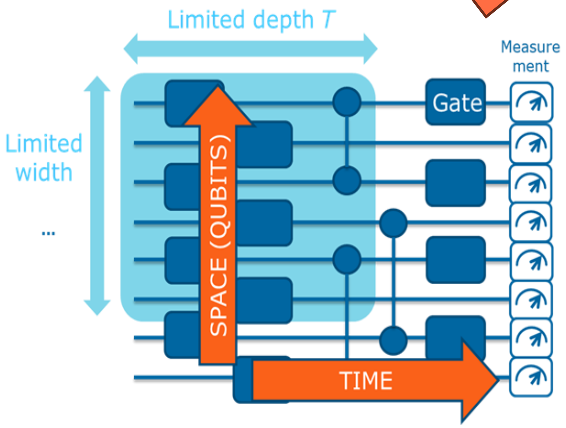

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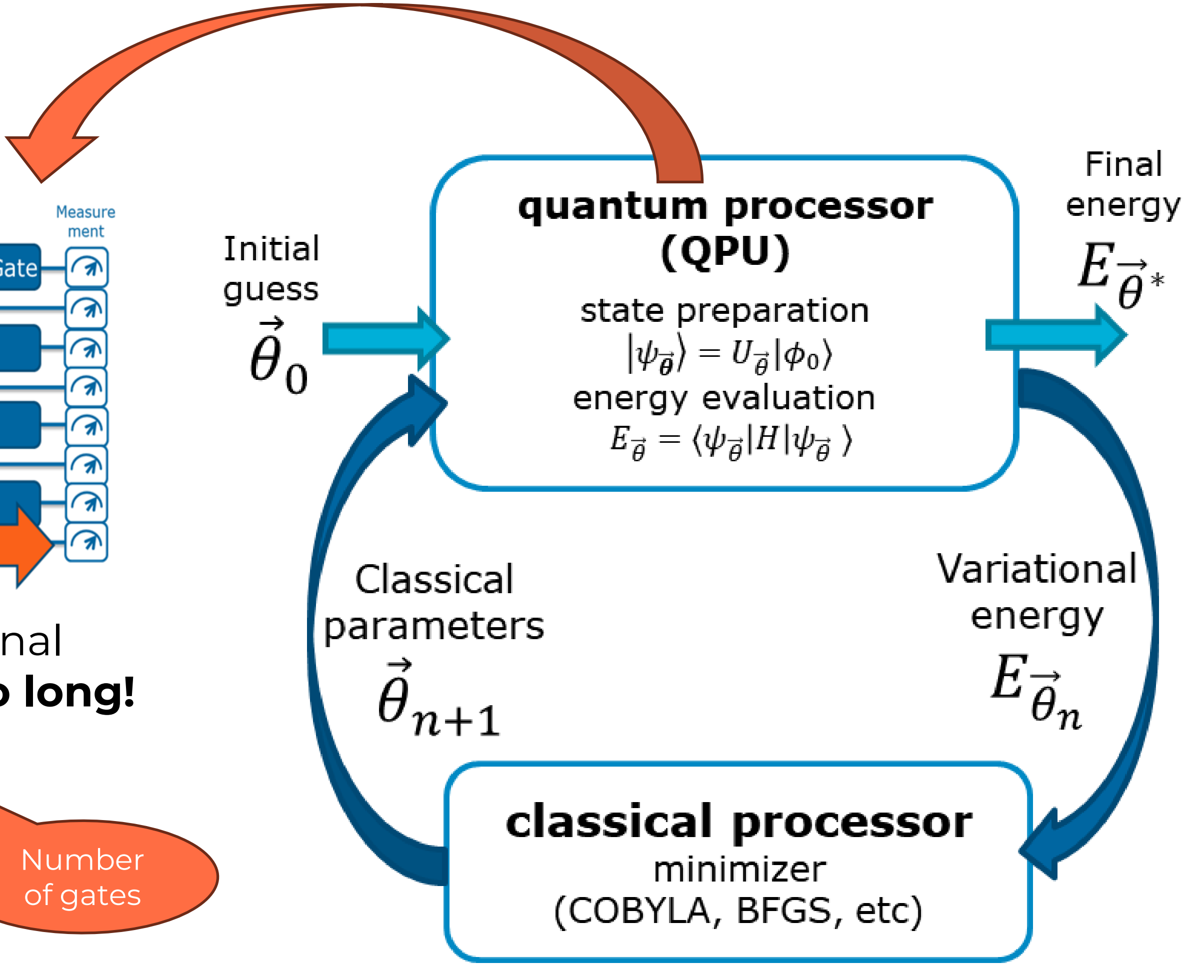

Electronic structure Hamiltonian:

$$H = \sum_{pq} h_{pq} c_p^\dagger c_q + \frac{1}{2}\sum_{pqrs} h_{pqrs} c_p^\dagger c_q^\dagger c_r c_s$$

Fermion antisymmetry:

$$c_4^\dagger|0010\rangle = -|0011\rangle$$

vs. qubits:

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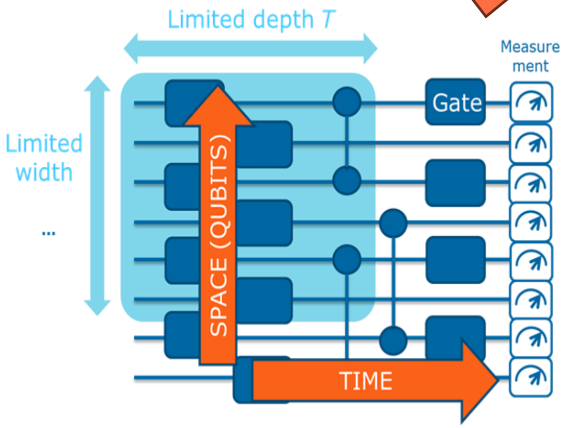

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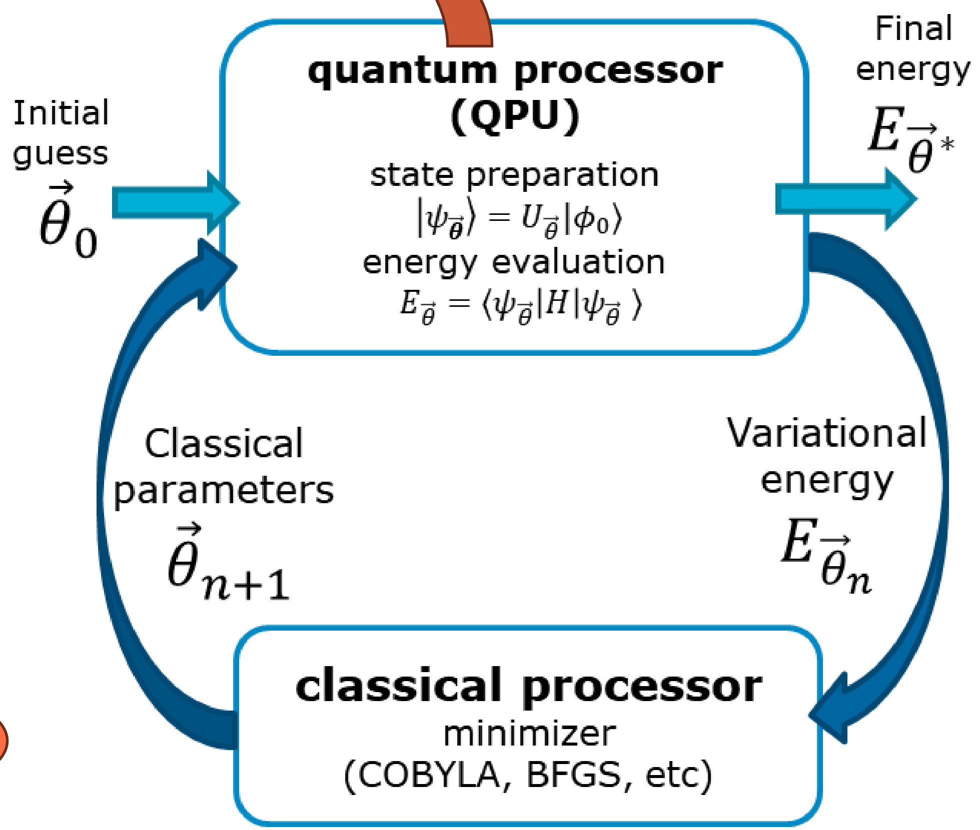

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Hence longer circuits!

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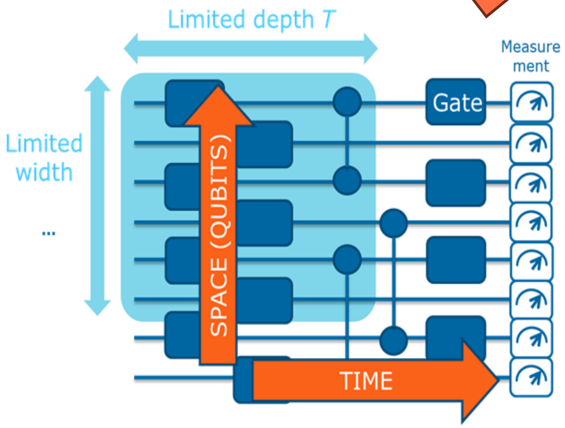

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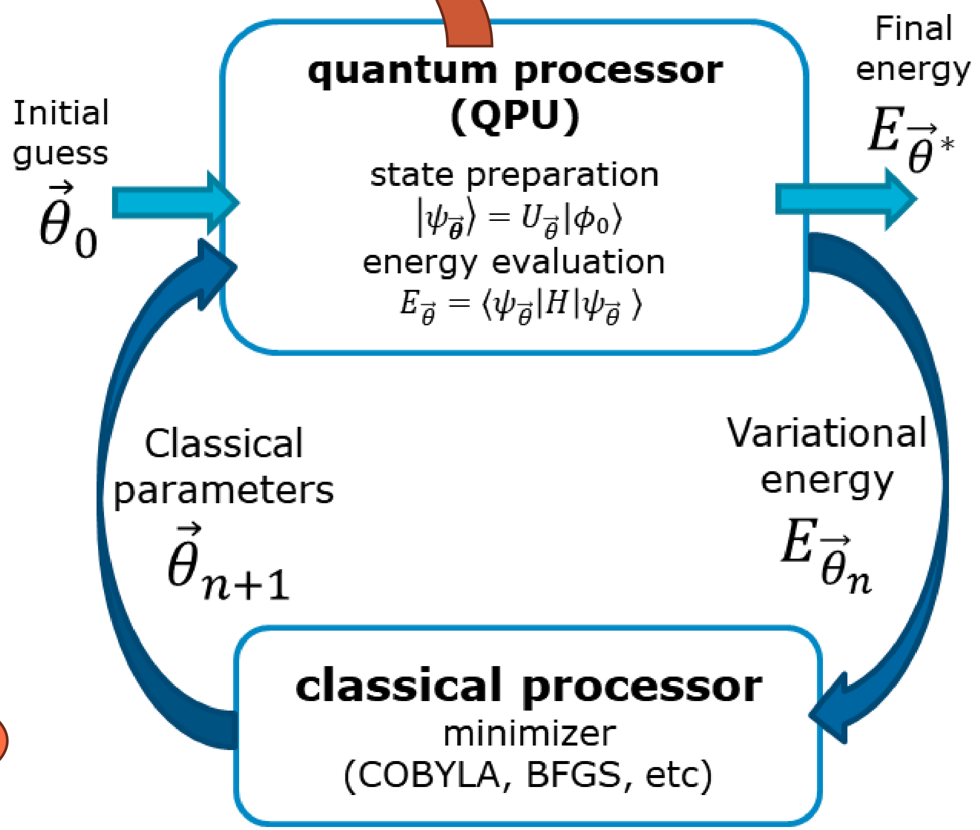

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Can we even avoid fermionic rules?

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Outline

- Can we shorten circuits?
- Can we even avoid fermionic rules?
- Hybridizing tensor networks and quantum algorithms
- Could we use quantum noise to our advantage?

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The importance of the orbital basis

Consider

$$H = \sum_{pq} h_{pq} c_p^\dagger c_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} c_p^\dagger c_q^\dagger c_r c_s$$

Hartree-Fock method: define

$$\tilde{c}_i^\dagger = \sum_p V_{ip} c_p^\dagger$$

Find orbital transformation V s.t HF wavefunction

$$|\Psi(V)\rangle = \tilde{c}_{i_1}^\dagger \cdots \tilde{c}_{i_{N_e}}^\dagger |00 \dots 0\rangle$$

minimizes $\langle\Psi(V)|H|\Psi(V)\rangle$

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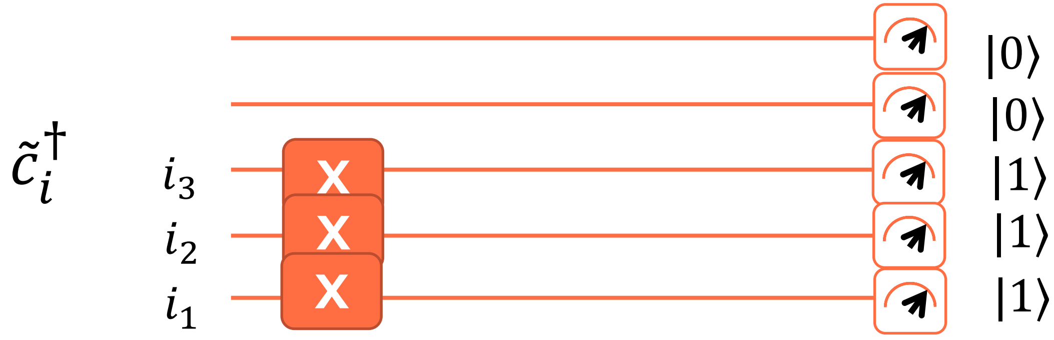
Quantum computer representation?

In $\tilde{c}_i^\dagger$ (molecular orbital) basis: $|\Psi(V)\rangle = \tilde{c}_{i_1}^\dagger \cdots \tilde{c}_{i_{N_e}}^\dagger |00 \ldots 0\rangle$



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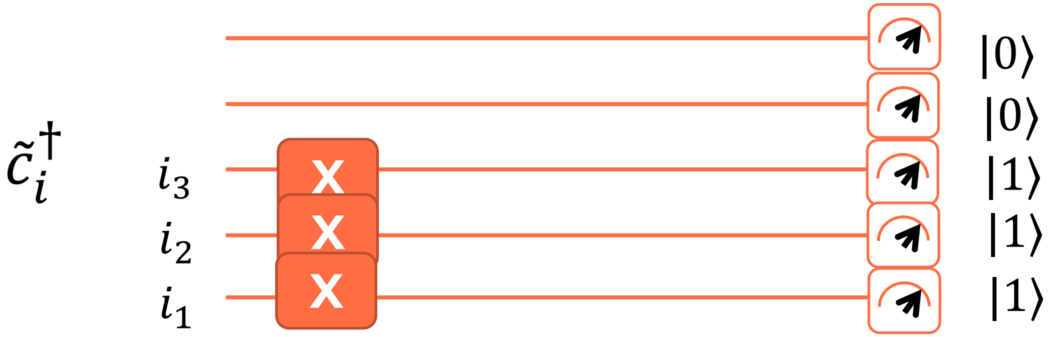
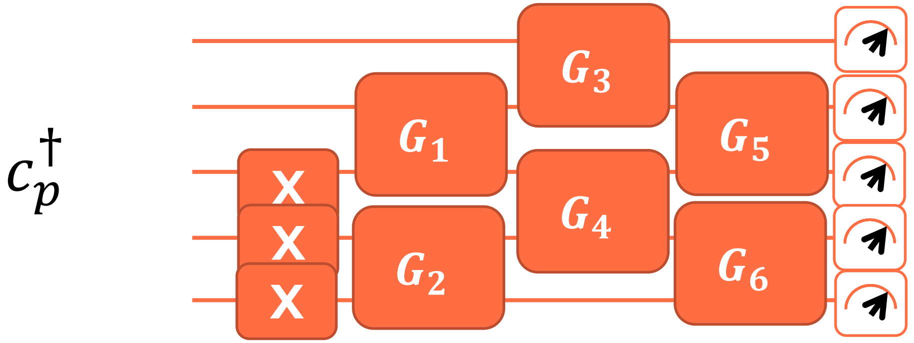


In e.g original basis… $|\Psi(V)\rangle$ much more complicated!



Cf Arute et al 2021

Givens rotations $\sim e^{hc^\dagger c}$… aka **Gaussian gates**

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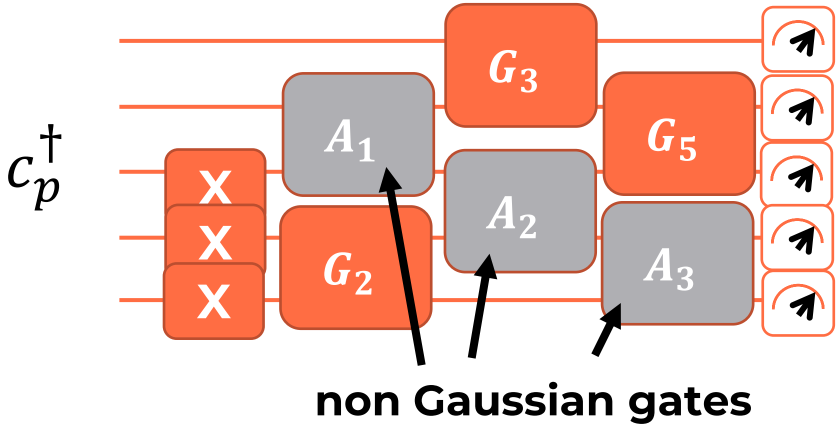
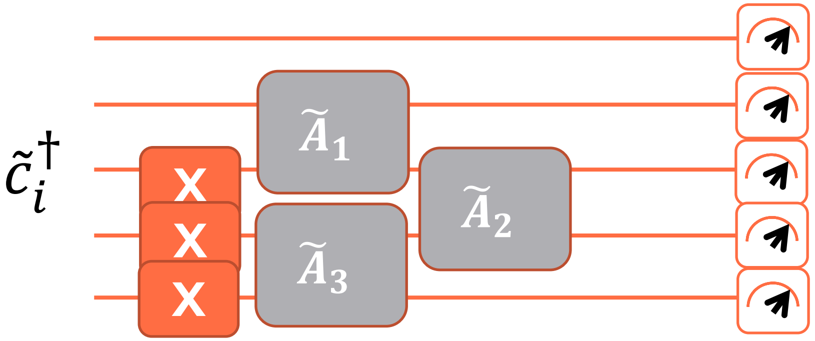
Beyond Hartree-Fock?

In original basis:



Can we find a (the?) basis that most simplifies the circuit?



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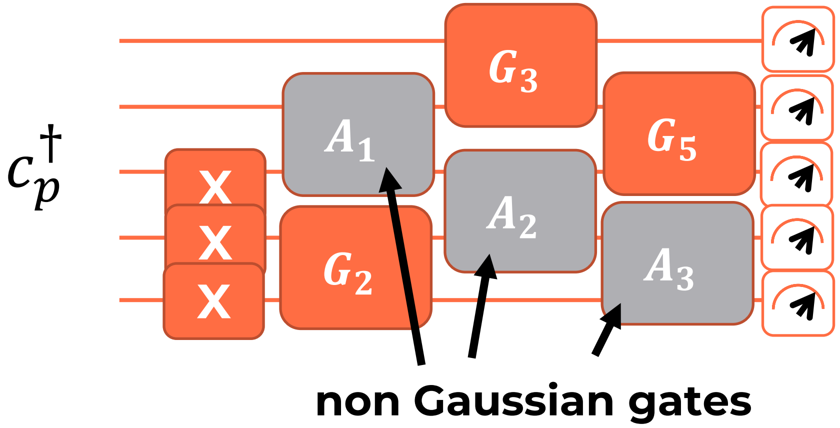

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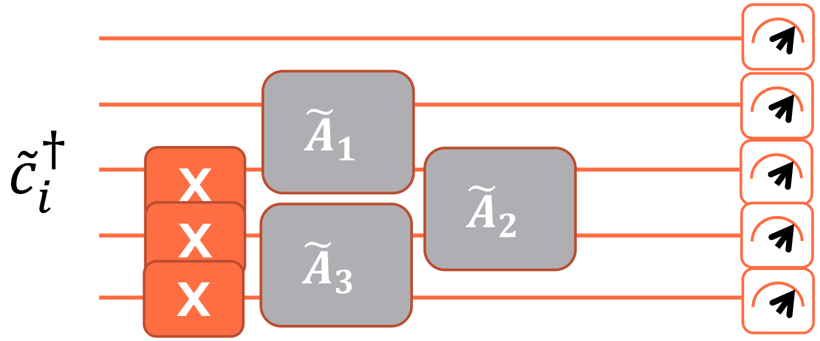


The natural orbital basis

The basis with fewest Slater determinants, hence shortest circuit!

How to compute it ?

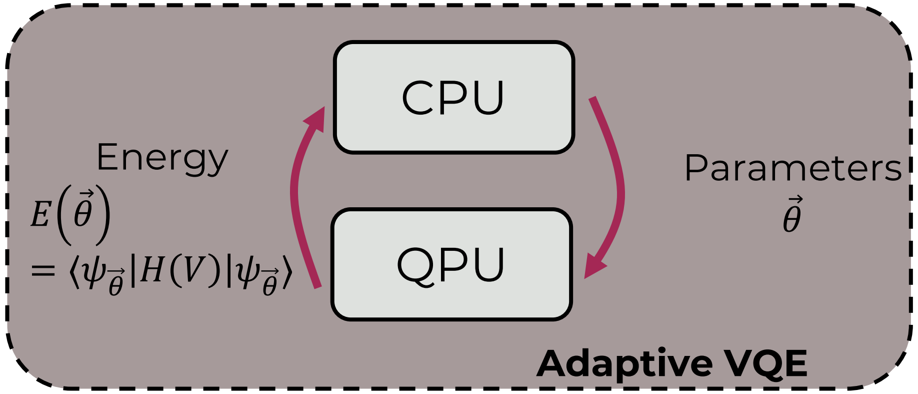
Diagonalize

$$D_{pq} = \langle \Psi | c_p^\dagger c_q | \Psi \rangle = V_{pi} n_i V_{iq}^\dagger$$

Iterative rotation to the natural orbital basis

Besserve, TA, PRB '22
Besserve, Ferrero, TA, 2406.14170

$|\Psi\rangle$ is unknown! Determine RDM iteratively



(Grimsley 2019)

See also: Koridon et al 2021 for orbital optimization

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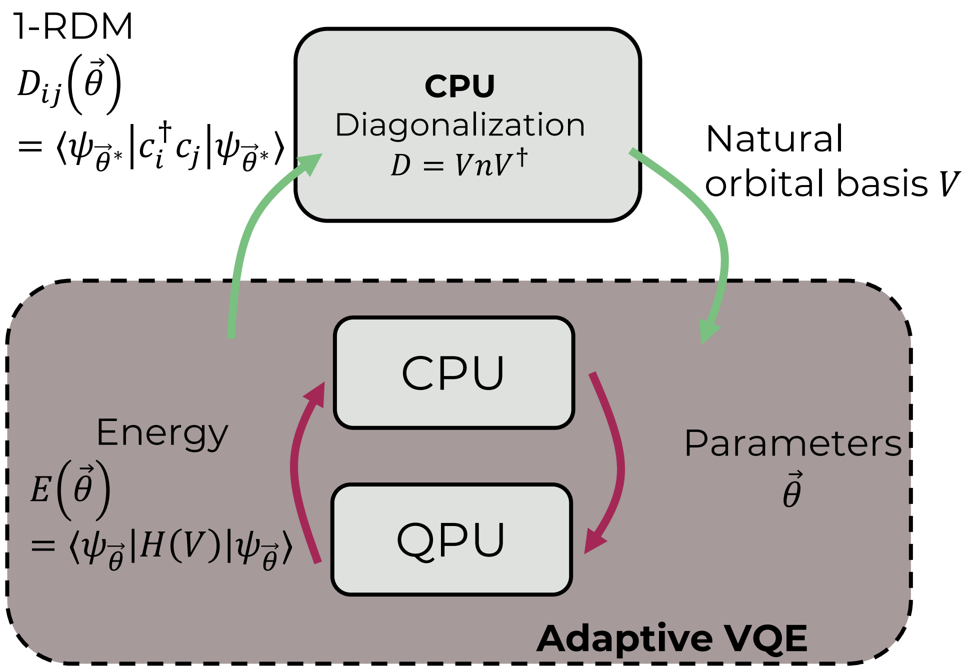

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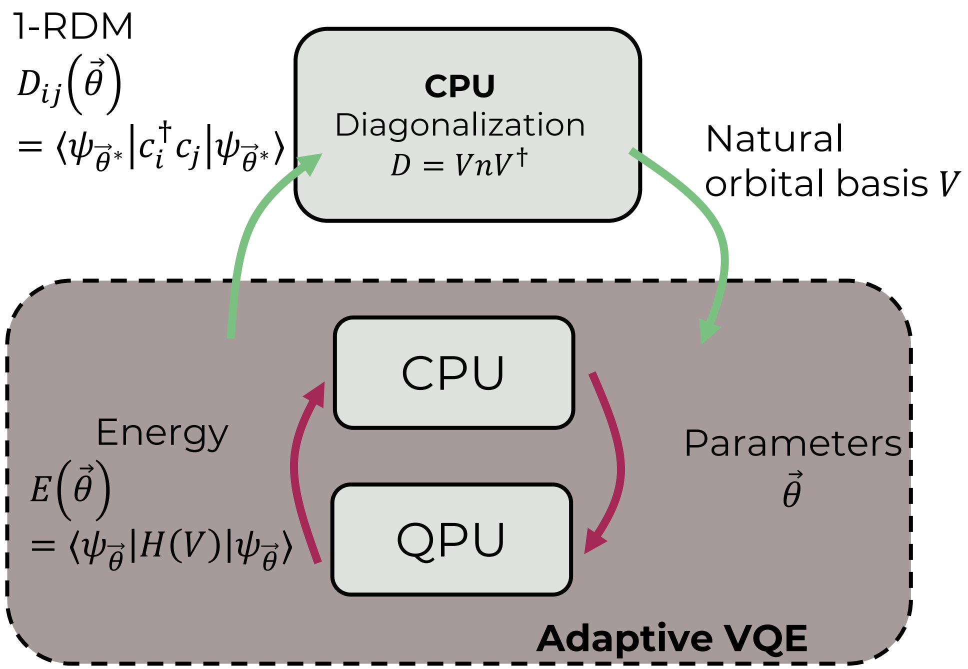

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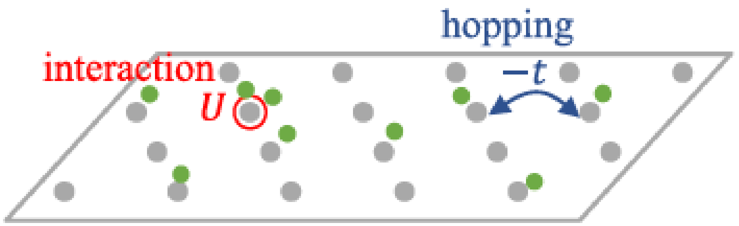
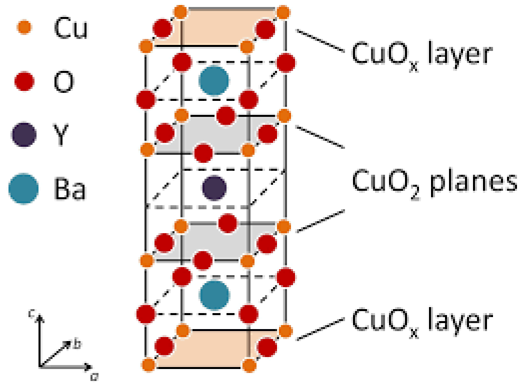
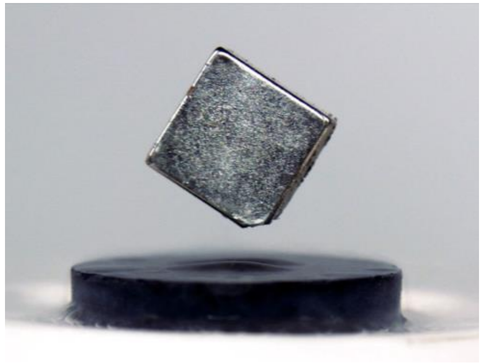
Application:
Hubbard model
(here N=2 sites):



Simplest model for high-temperature superconductors





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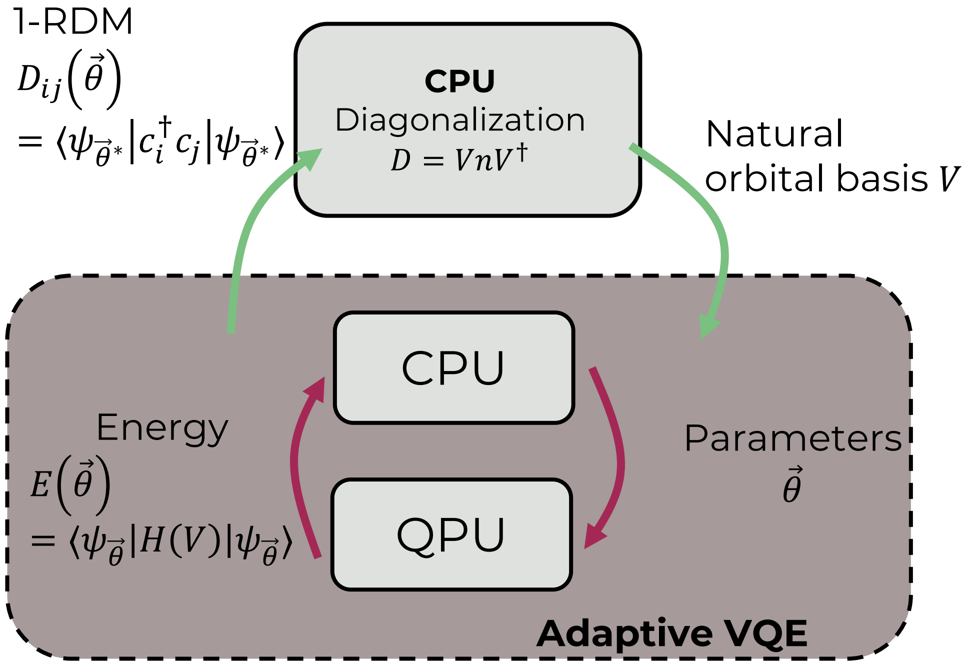

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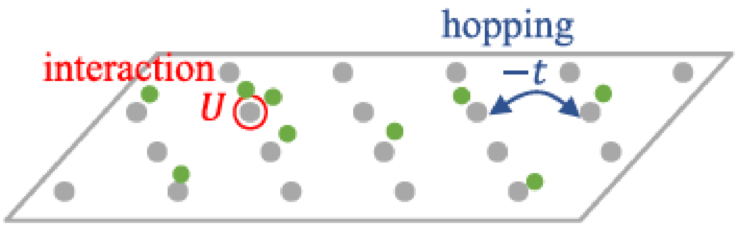

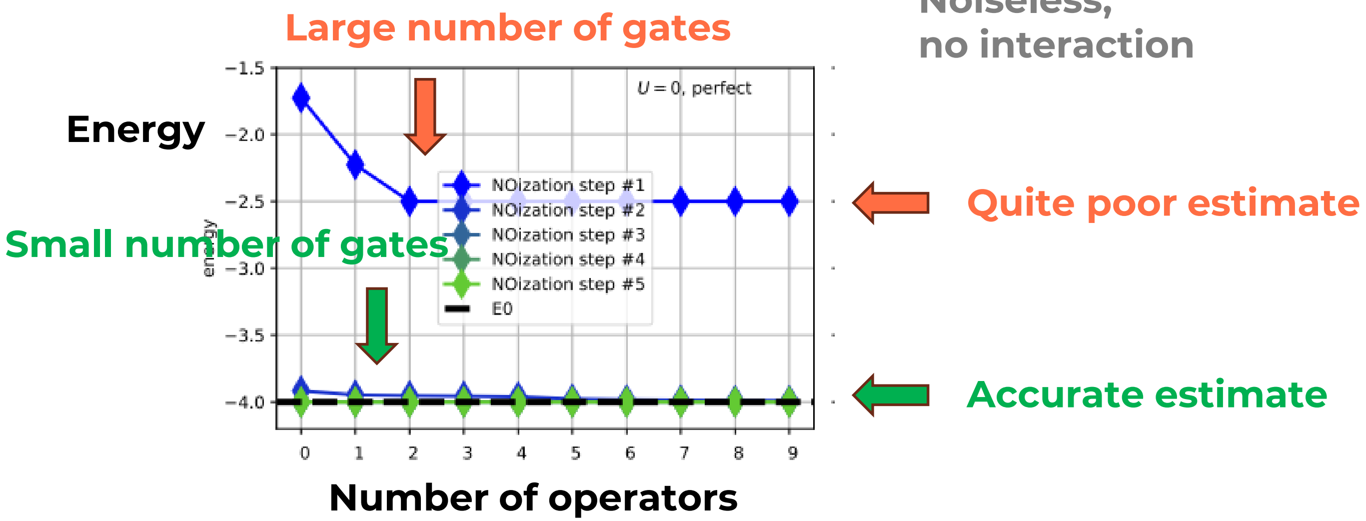

See also: Koridon et al 2021 for orbital optimization

Conclusions of Part 1

One method to reduce sensitivity to decoherence.

Still many issues with VQE (even without noise!)

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(Wecker 2017)

- Barren plateau problem (McClean 2018)

$\sigma(E) \sim \frac{1}{2^n}$

Ways out?

- Clever initialization
- Change way of optimizing
- (etc)

Find zeroes instead of minimizing: the projective quantum eigensolver (PQE)

Plazanet, TA, 2410.15129

Chemistry: Unitary Coupled Cluster ansatz $U\left(\vec{\theta}\right)|\mathrm{HF}\rangle$

VQE: minimize $\langle HF|U^{\dagger}\left(\vec{\theta}\right)HU\left(\vec{\theta}\right)|\mathrm{HF}\rangle$

PQE: find zeros of 'residues':

Stair et al '22

$$r_{\mu}\left(\vec{\theta}\right) = \langle \mathrm{EX}_{\mu}|U^{\dagger}\left(\vec{\theta}\right)HU\left(\vec{\theta}\right)|\mathrm{HF}\rangle$$

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Root finding: Newton-Raphson algorithm

- Convergence guarantees! (Newton-Kantorovitch theorem)
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EVIDEN

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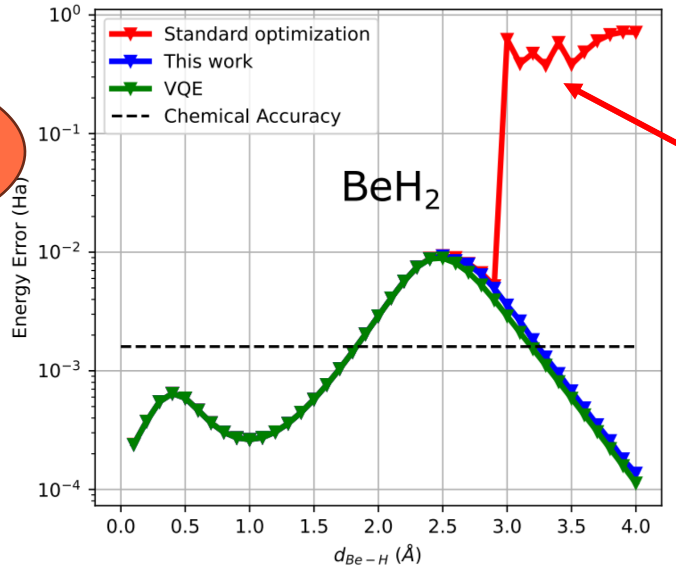

New hybrid update rule (GD+Newton)

➔ Better convergence than **standard PQE**

➔ Similar to **VQE** (but with error estimation)

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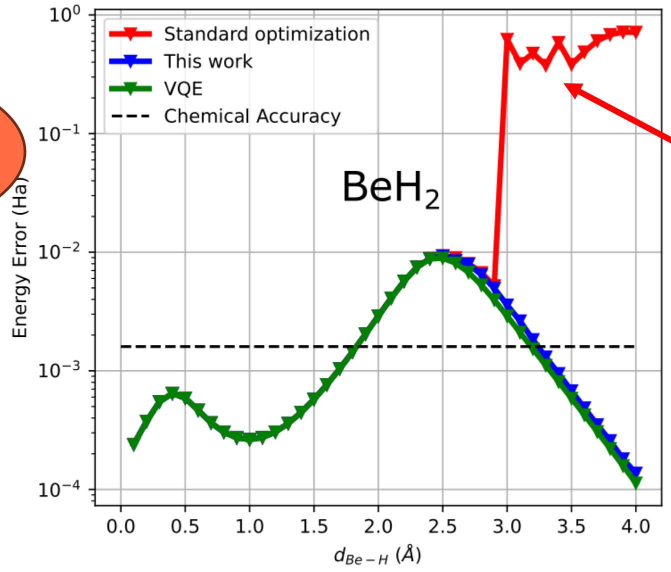

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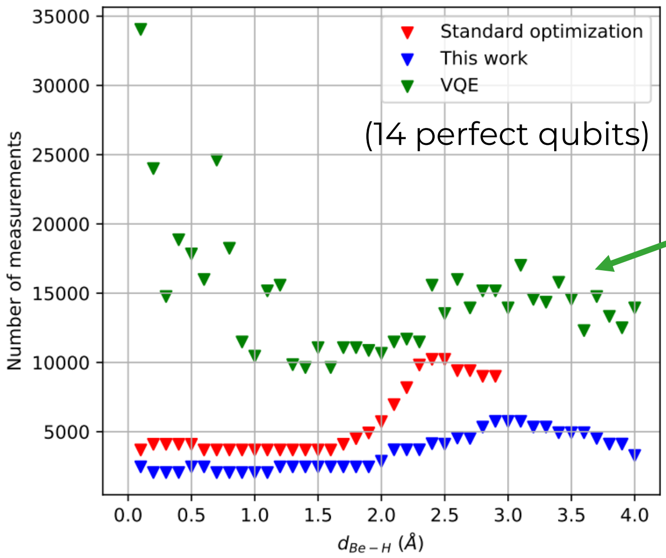


→ Much fewer measurements than **VQE**.

→ Can it help mitigate barren plateau issue?

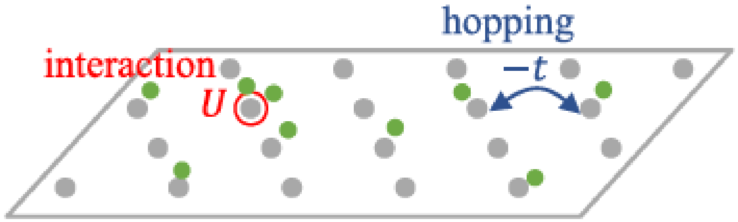
EVIDEN

Outline

- Can we shorten circuits?
- **Can we even avoid fermionic rules?**
  Hubbard physics with Rydberg processors
- Hybridizing tensor networks and quantum algorithms
- Could we use quantum noise to our advantage?

Mott physics in the Hubbard model

2D Hubbard model

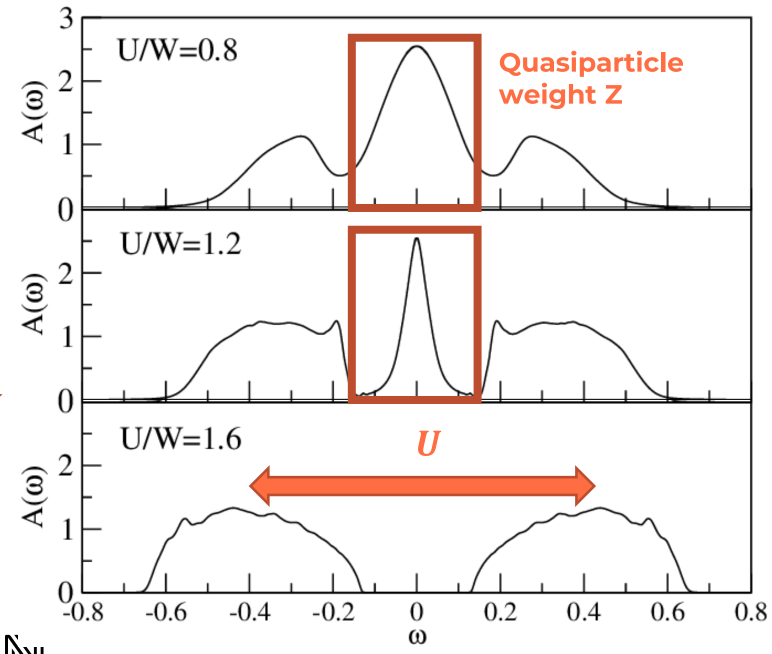


Typical evolution of the spectral function:

Fermi liquid

More interactions

Mott insulator



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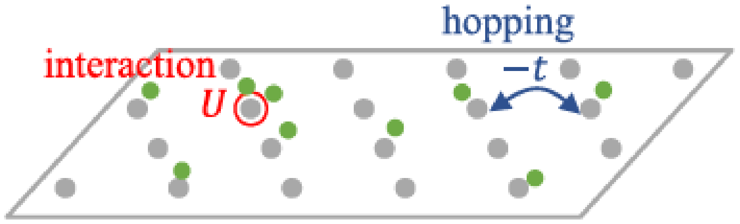

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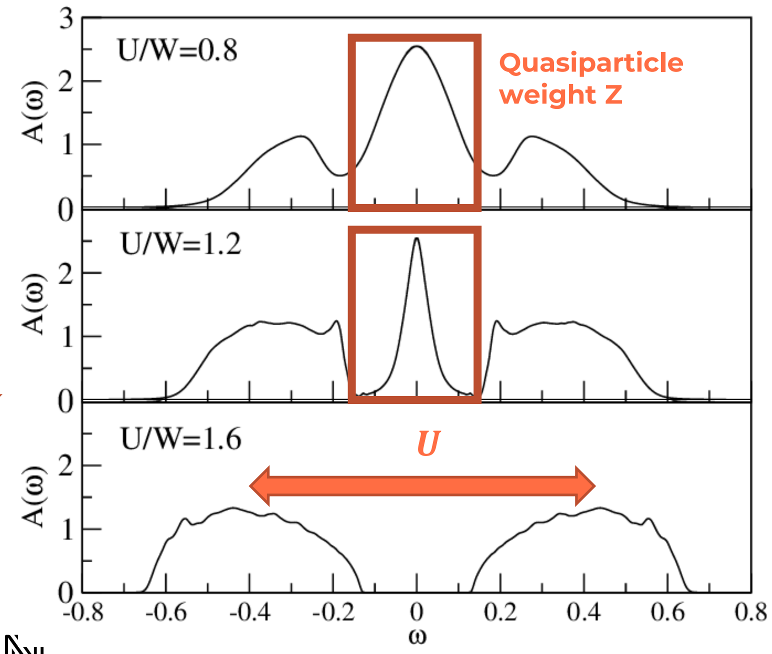
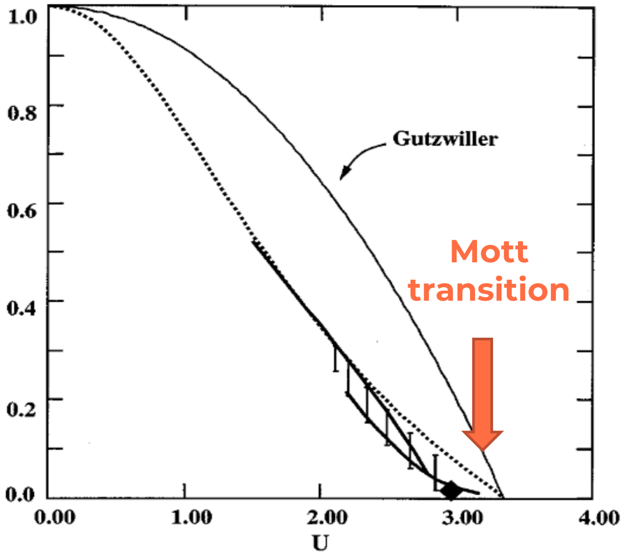


Equilibrium properties:
Mott transition

Quasiparticle weight Z



DMFT
Georges et al '96

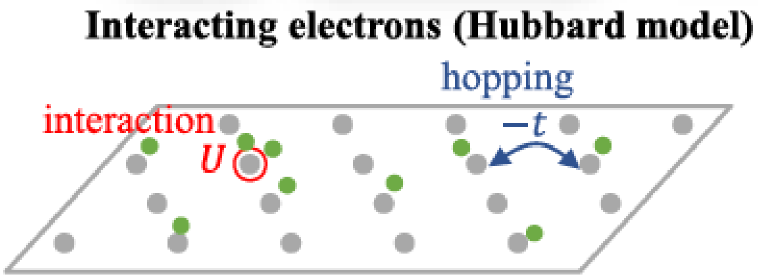
EVIDEN

Mott physics on spin-based quantum processors

Michel, Henriet, Domain, Browaeys, TA, PRB 24

Goal: avoid overhead of fermion-to-qubit translation

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



"Slave-spin theory": decompose

$$c_{i\sigma}^{\dagger} = Z_i f_{i\sigma}^{\dagger}$$

spin

pseudo-fermion

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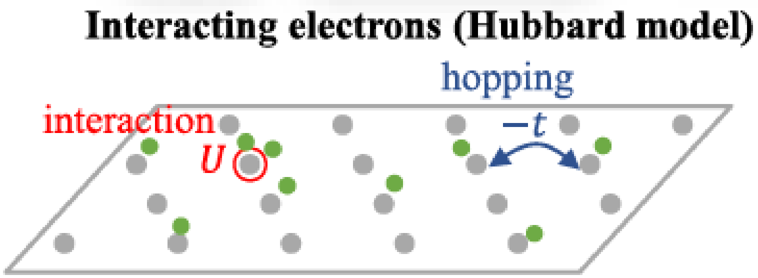

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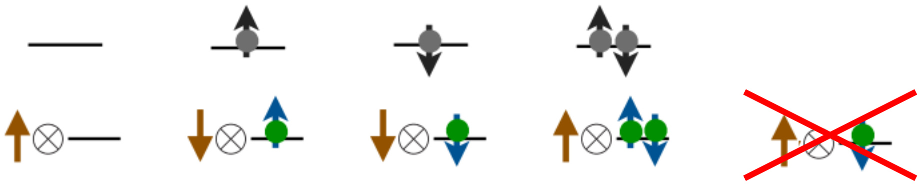
Larger Hilbert space: only a smaller subspace is physical:



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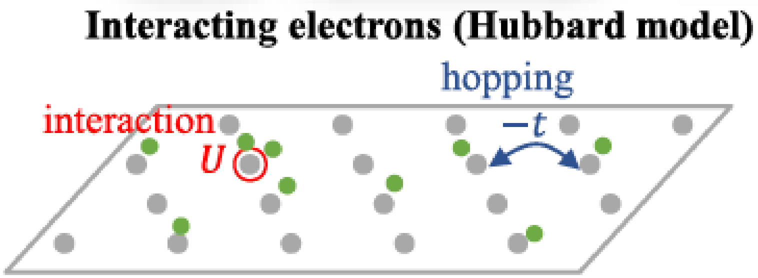

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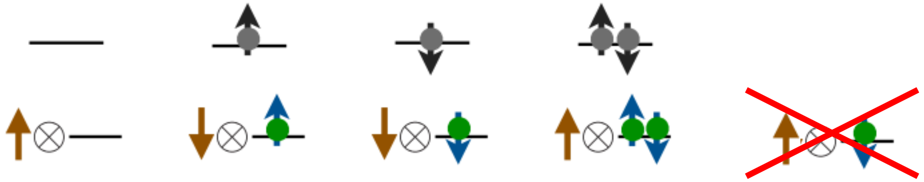

Approximation: Mean-field decoupling:

$$Z_i Z_j f^\dagger_{i\sigma} f_{j\sigma} \approx \langle Z_i Z_j \rangle f^\dagger_{i\sigma} f_{j\sigma} + Z_i Z_j \langle f^\dagger_{i\sigma} f_{j\sigma} \rangle + const.$$

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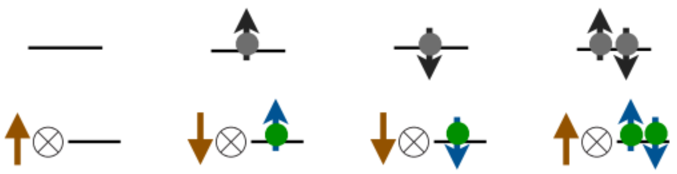

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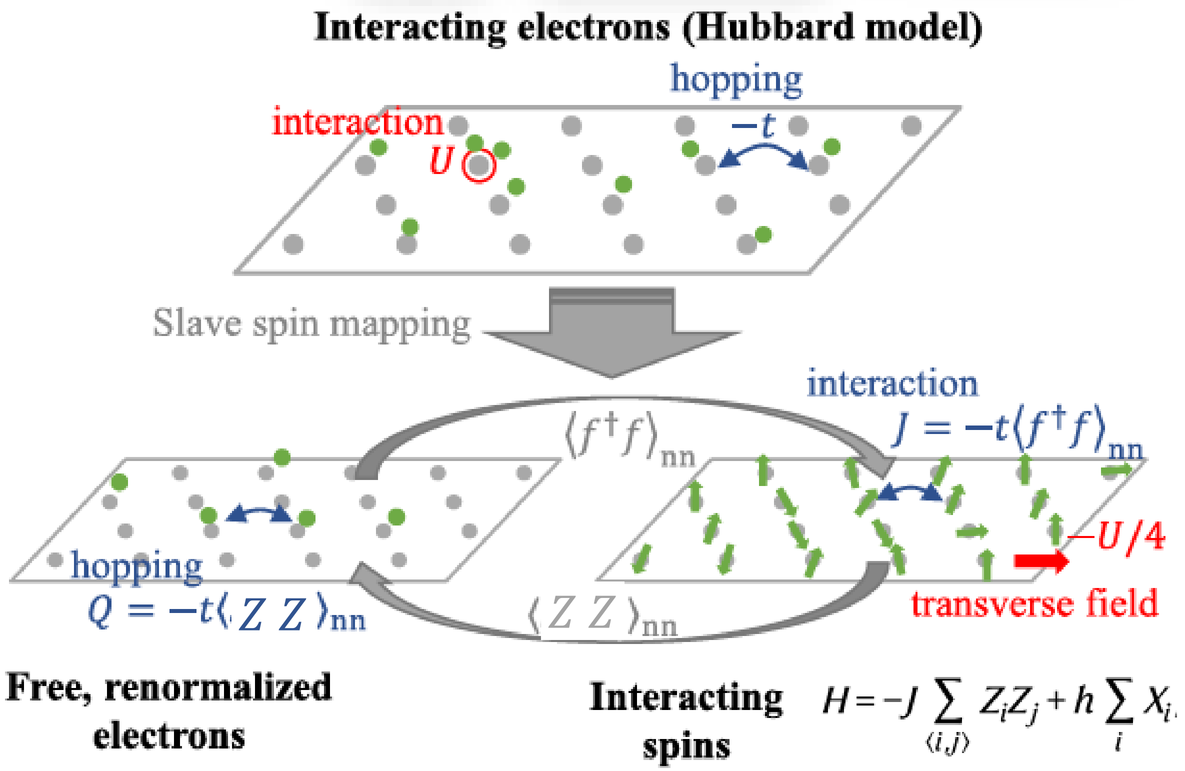

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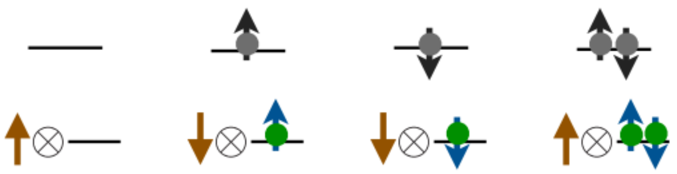

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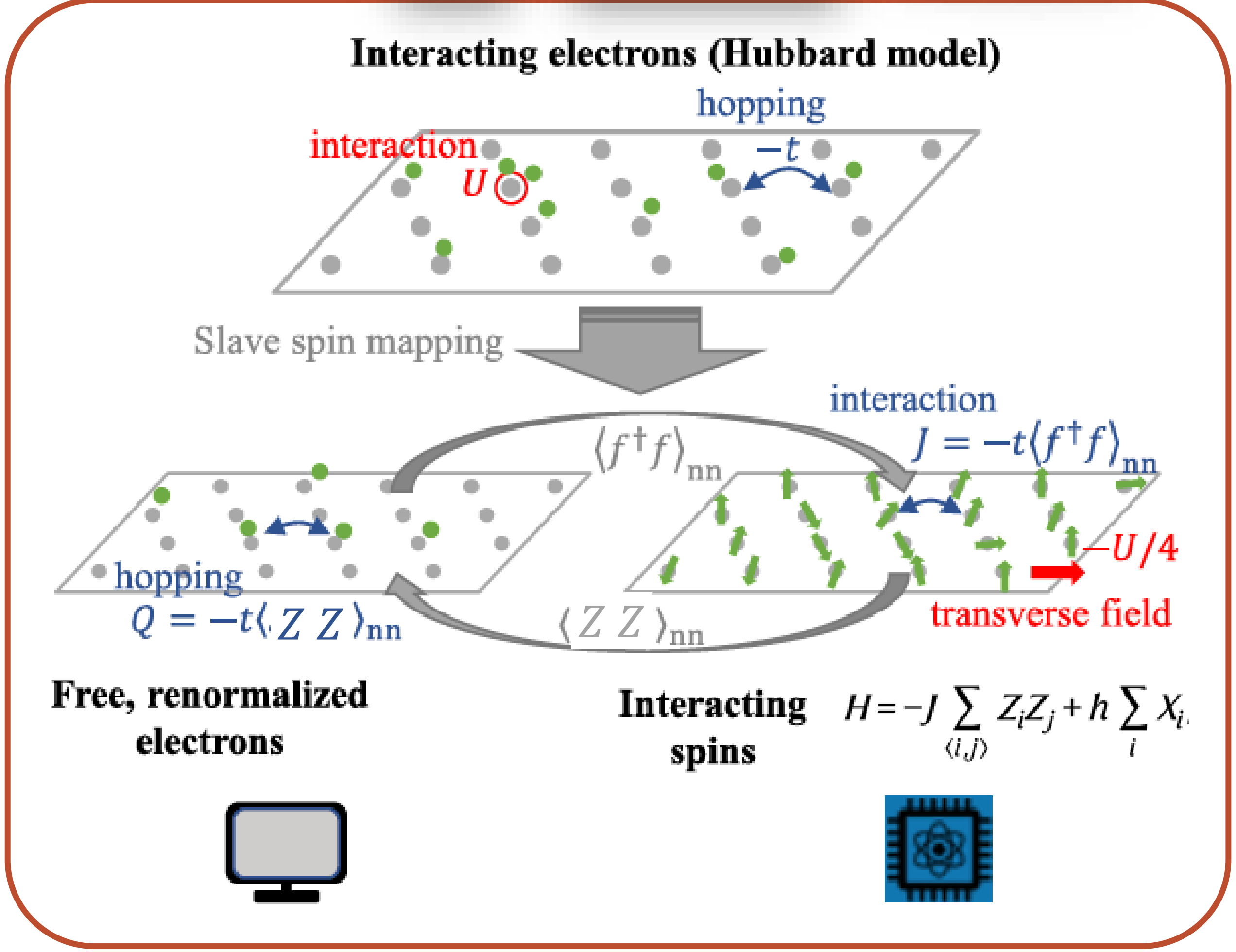

Using Rydberg atoms to deal with the spin model

Michel, Henriet, Domain, Browaeys, TA, PRB 24

Effective model: Transverse Field Ising model (TFIM):

$$H_{\mathrm{s}}^{\mathcal{C}} = \sum_{i,j\in\mathcal{C}} J_{ij} S_i^z S_j^z + \frac{U}{4}\sum_{i\in\mathcal{C}} S_i^x + \sum_{i\in\mathcal{C}} h_i S_i^z,$$

… very close to Rydberg atom Hamiltonian!

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Review: Browaeys & Lahaye 2020

EVIDEN

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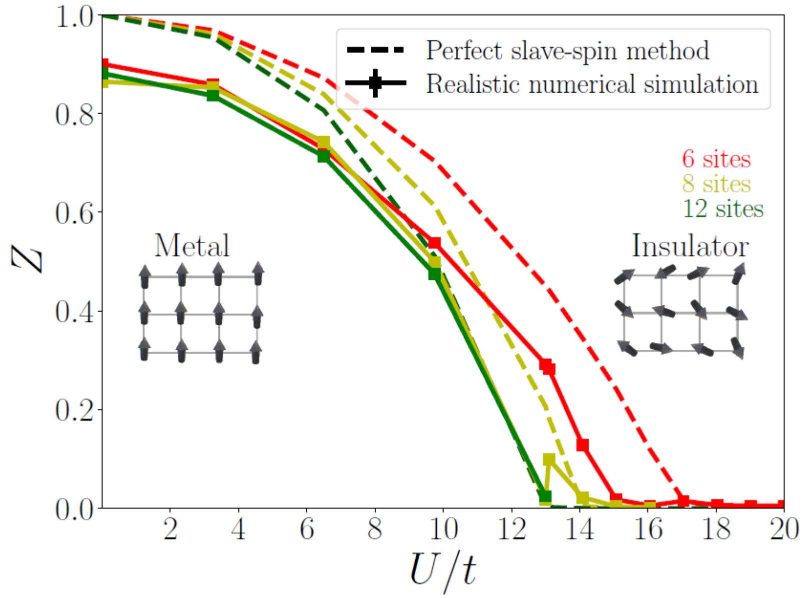

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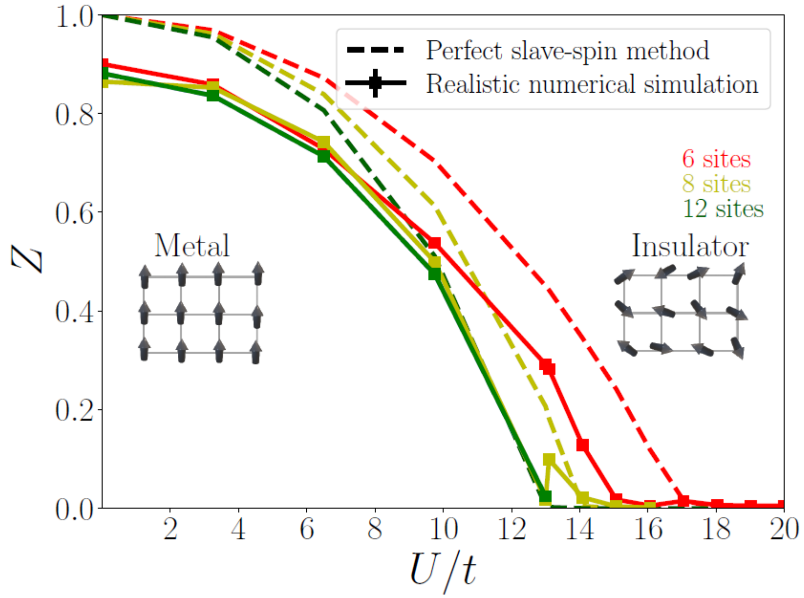

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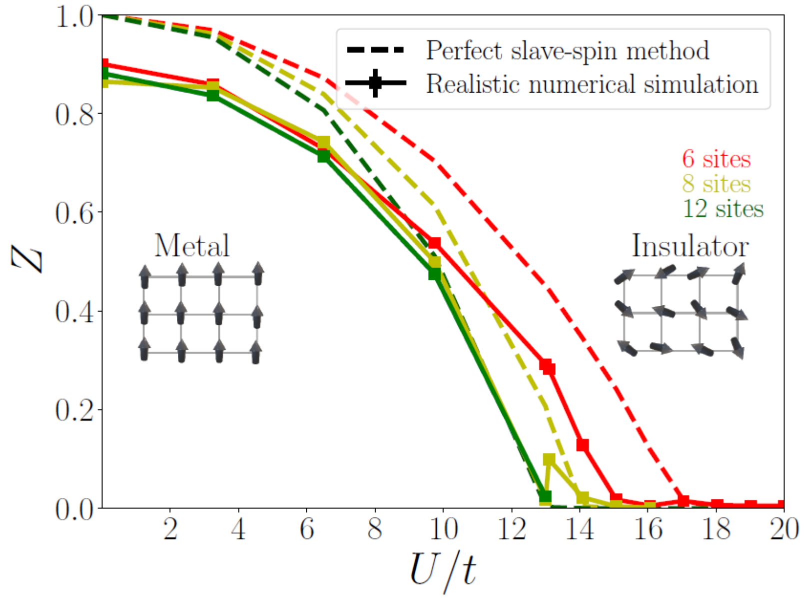

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Ongoing experimental realization @Pasqal!

EVIDEN

EVIDEN

Outline

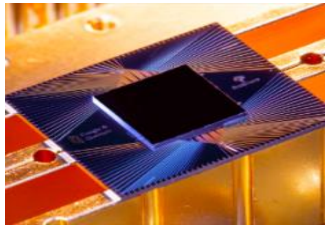
- Can we shorten circuits?
- Can we even avoid fermionic rules?
  Hubbard physics with Rydberg processors
- **Hybridizing tensor networks and quantum algorithms**
  Jump-starting quantum computations
- Could we use quantum noise to our advantage?

Google's and IBM's quantum advantage claims

Google supremacy?

(Arute et al '19)

Sycamore, 53 qubits



Sampling from random circuits

200 seconds! (and $F = 0.2\%$!)

classical emulation: 10,000 years

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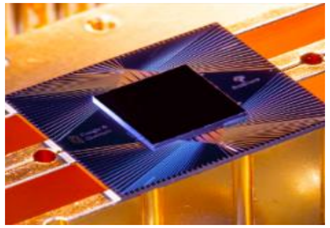

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What happened?

TA et al, PRXQ 2023

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Morvan et al '23

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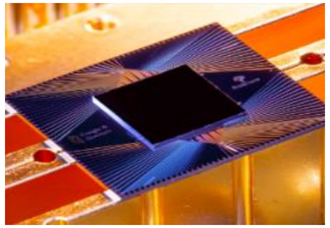

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Morvan et al '23

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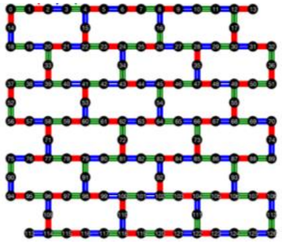
IBM useful advantage?

(Kim et al '23)

Eagle, 127 qubits



Quench on transverse Ising model

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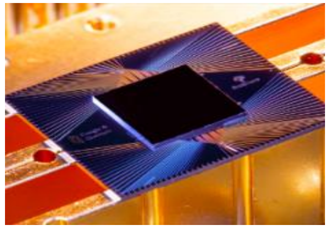


Sampling from random circuits

200 seconds! (and $F = 0.2\%$!)

classical emulation: ~~10,000 years~~

What happened?

TA et al, PRXQ 2023

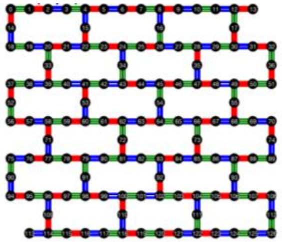
Exp.	1 amp.	1 million noisy samples		
	FLOPs	FLOPs	XEB fid.	Time
SYC-53 [9]	$6.44 \cdot 10^{17}$	$2.60 \cdot 10^{17}$	$2.24 \cdot 10^{-3}$	6.18 s

Morvan et al '23

IBM useful advantage?

(Kim et al '23)

Eagle, 127 qubits



Quench on transverse Ising model

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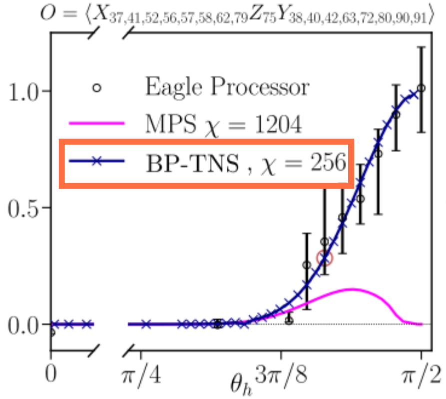

Classical emulation:
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Google's and IBM's quantum advantage claims

Google supremacy?

(Arute et al '19)

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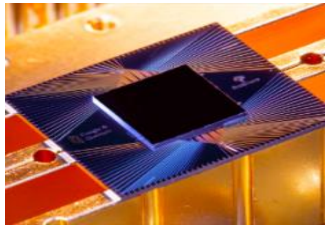

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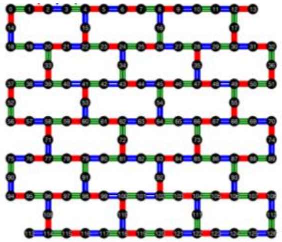

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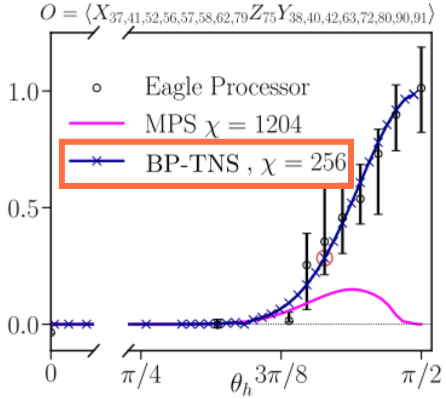

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Method to beat the exponential wall?

Basics of tensor networks (matrix product states)

Generic wavefunction:

$$|\Psi\rangle = \sum_{b_1 b_2 \ldots b_n} \psi_{b_1 b_2 \ldots b_n} |b_1, \ldots, b_n\rangle$$

Storage cost

Representation:

$$\psi_{b_1 b_2 b_3} =$$

2^n

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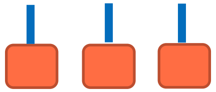

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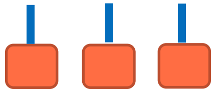
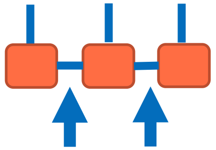
If no entanglement, $\psi_{b_1 b_2 \ldots b_n} = \psi_{b_1} \phi_{b_2} \varphi_{b_3}$ $\quad \psi_{b_1 b_2 b_3} =$  $2n$

If some entanglement: $\psi_{b_1 b_2 b_3} = \mathrm{Tr}\left(A_{b_1} B_{b_2} C_{b_3}\right)$ $\quad \psi_{b_1 b_2 b_3} =$  $2n\chi^2$

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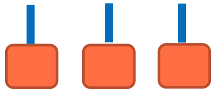
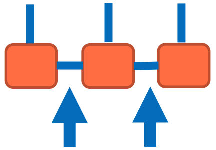
If no entanglement, $\psi_{b_1 b_2 \dots b_n} = \psi_{b_1} \phi_{b_2} \varphi_{b_3}$ $\qquad \psi_{b_1 b_2 b_3} =$  $2n$

If some entanglement: $\psi_{b_1 b_2 b_3} = \mathrm{Tr}\left(A_{b_1} B_{b_2} C_{b_3}\right)$ $\qquad \psi_{b_1 b_2 b_3} =$  $2n\chi^2$

Bond dimension χ

No free lunch: if entanglement S, **need**

$$\chi \gtrsim 2^S$$

1 exponential wall + 1 exponential wall < 2 exponential walls?

Tensor network (TN) showstopper:

Need $\chi \gtrsim 2^S$

with S : entanglement entropy

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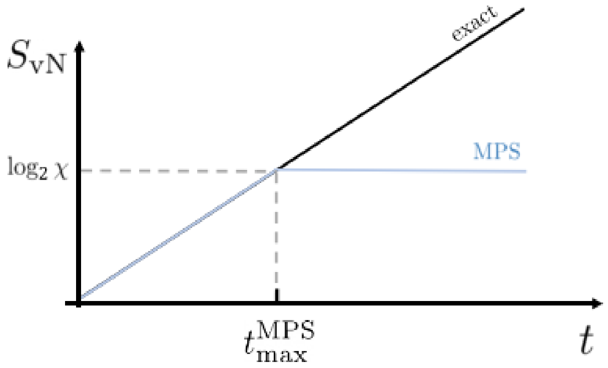

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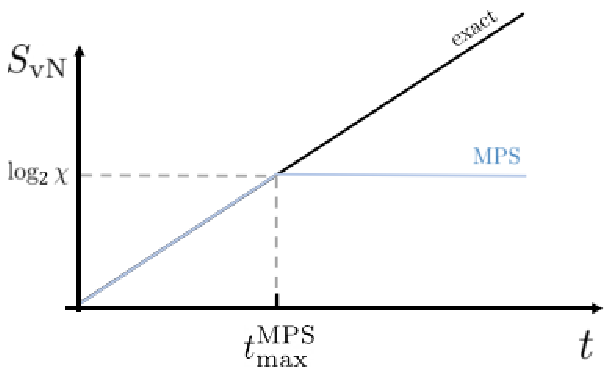

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Fidelity reduction $F \propto e^{-pN_g}$

Large N_g for accurate Suzuki-Trotter time evolution:

$$e^{-iHt} = \prod_k^{N_t} \prod_{\langle ij \rangle} R_{ZZ}(ij) \prod_i R_X(i) + O\left(\frac{t}{N_t}\right)^2$$

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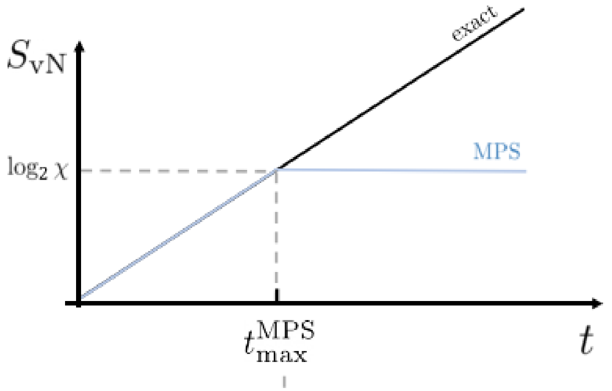

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Two key ideas:

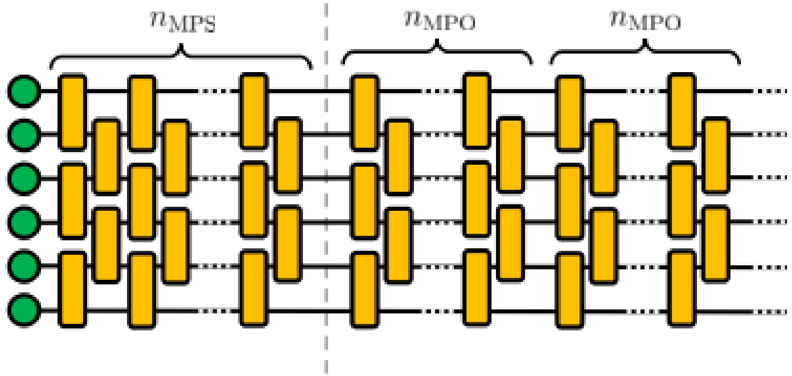
⇒ Push TN computation to its limit and take over with QC

⇒ Use TN techniques to compress quantum circuits

Hybridizing tensor networks and quantum computation

Anselme-Martin, TA et al, PRA 24
See also Causer et al '23

Formal target: fine-grained Suzuki-Trotter time evolution:



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Too many steps for QC (limited coherence)

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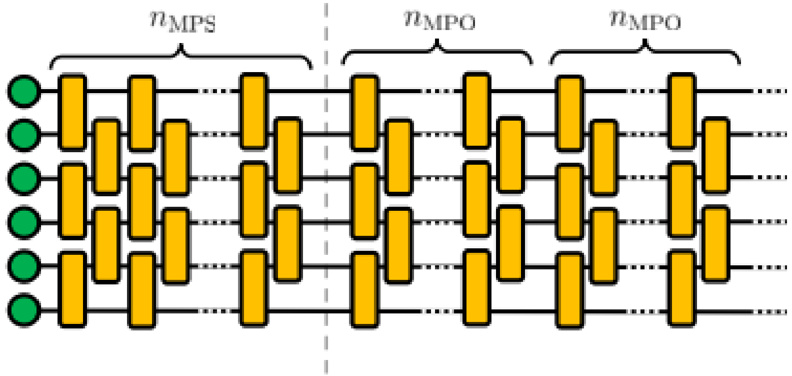

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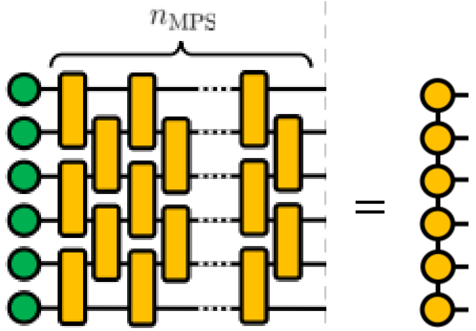
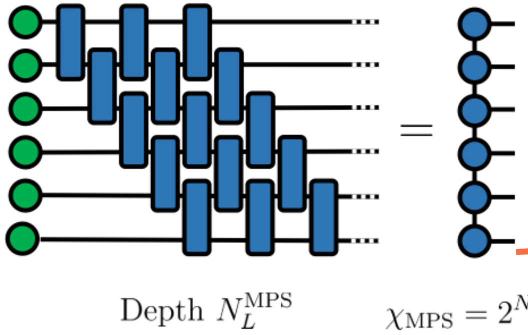


QMPS circuit ansatz:



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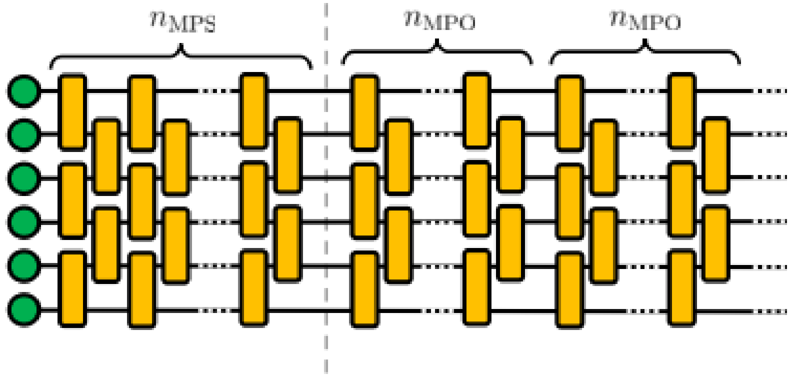

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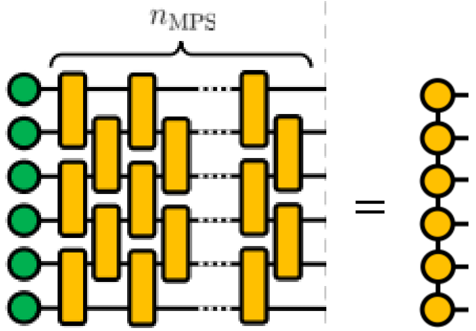

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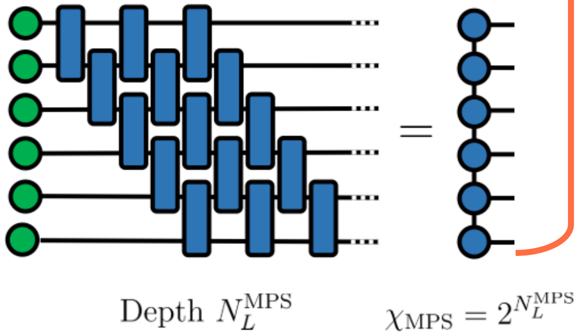

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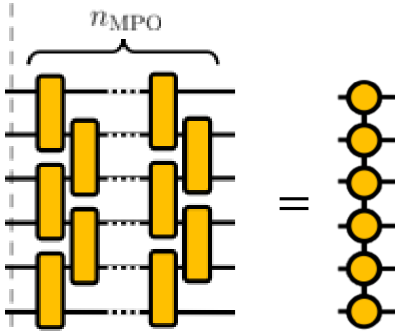

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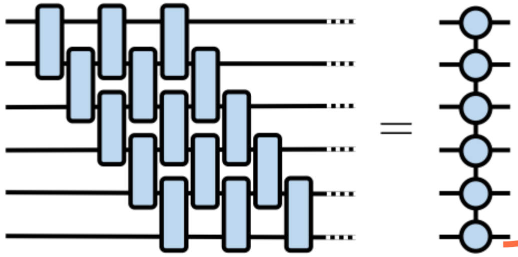

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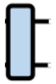

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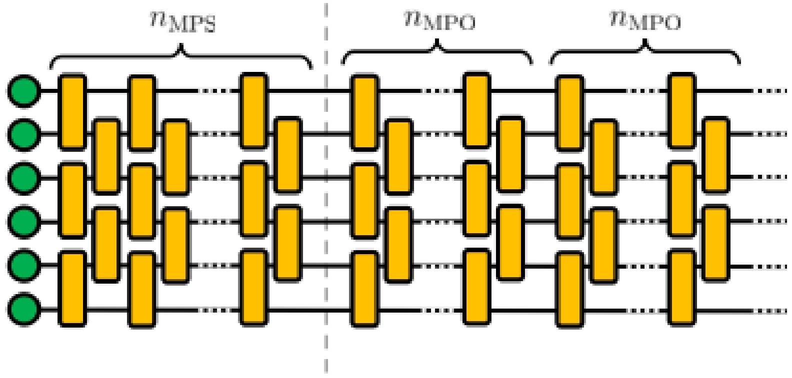

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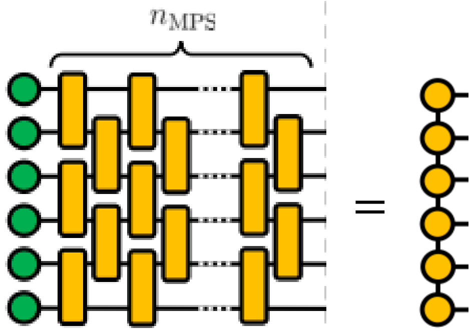

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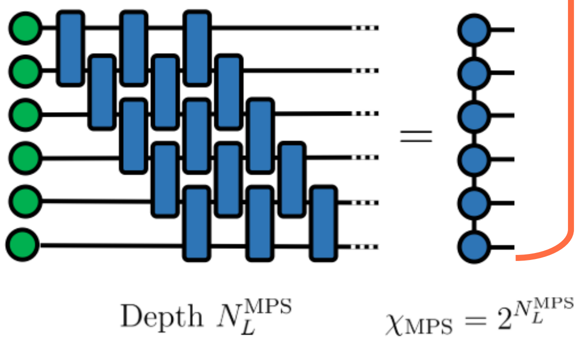

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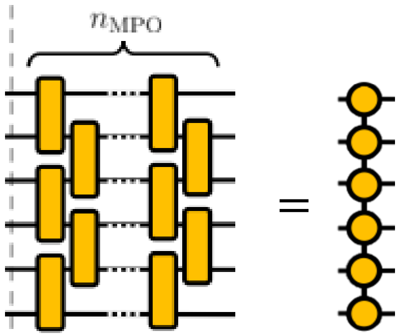

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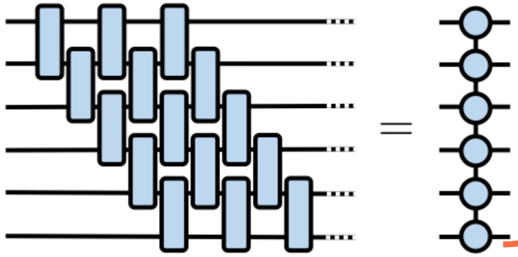

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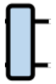

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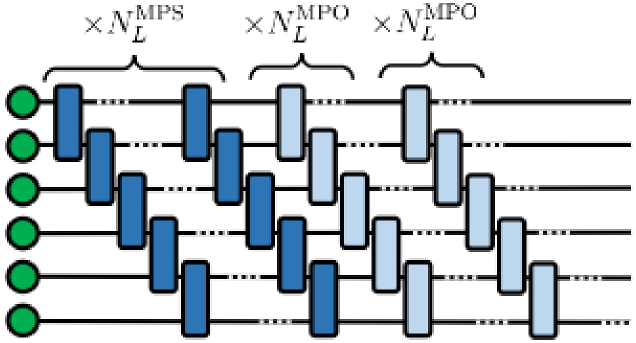

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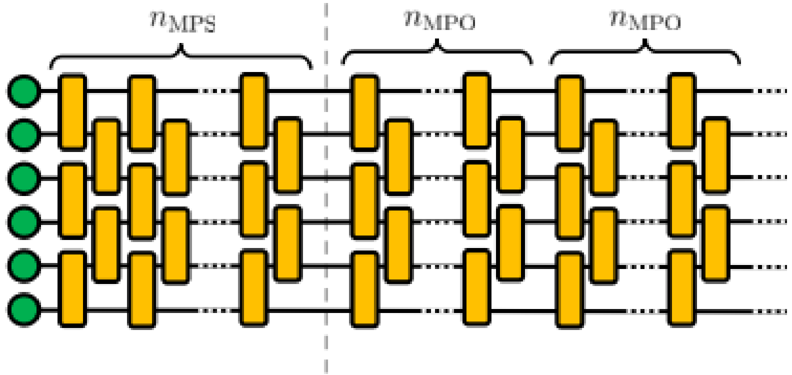

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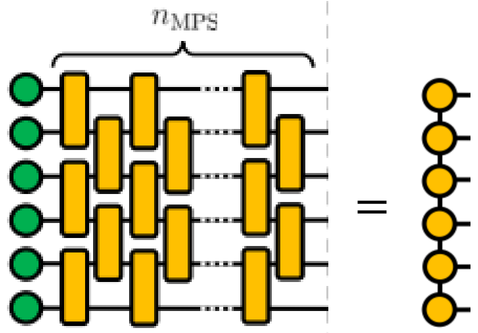

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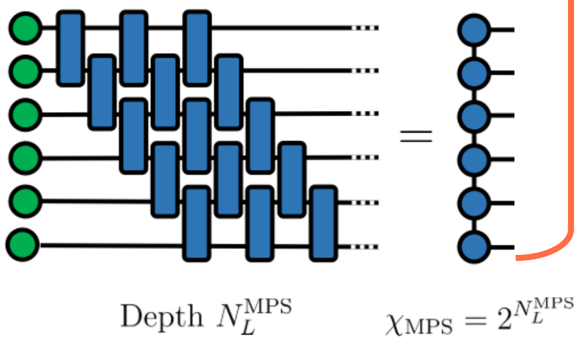

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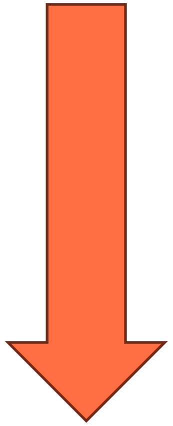

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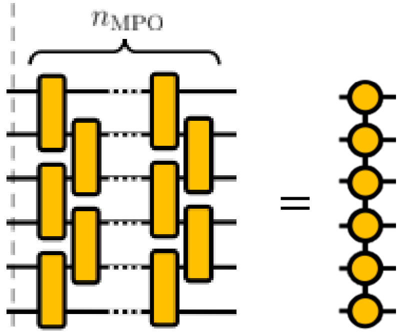

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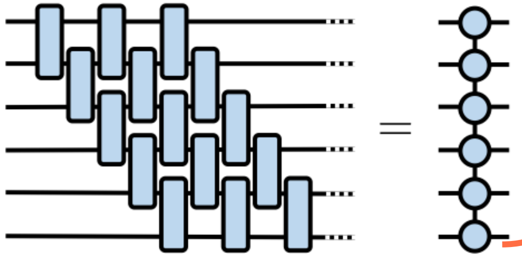

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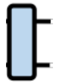

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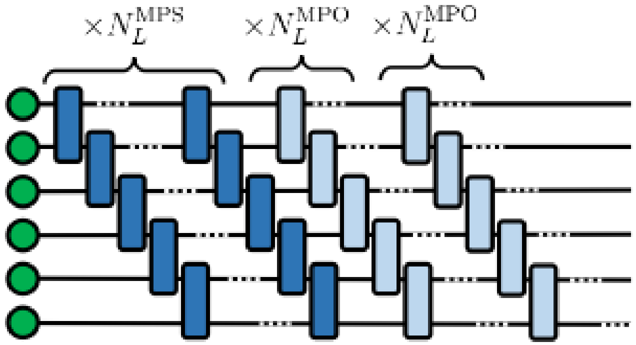

What did we gain?

$$N_L^{MPS} \ll n_{MPS}$$
$$N_L^{MP0} \ll n_{MP0}$$

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Experimental proof of concept on IBM quantum computers

Anselme-Martin, TA et al, PRA 24
See also Causer et al '23

Look at magnetization for quenched Ising

$$H = -J \sum_{\langle i,j \rangle} Z_i Z_j + h \sum_i X_i,$$

- 10 spins/qubits (toy model)
- Assume fixed RAM, hence max bond dim
  $\Rightarrow$ max time to keep MPS 'exact'

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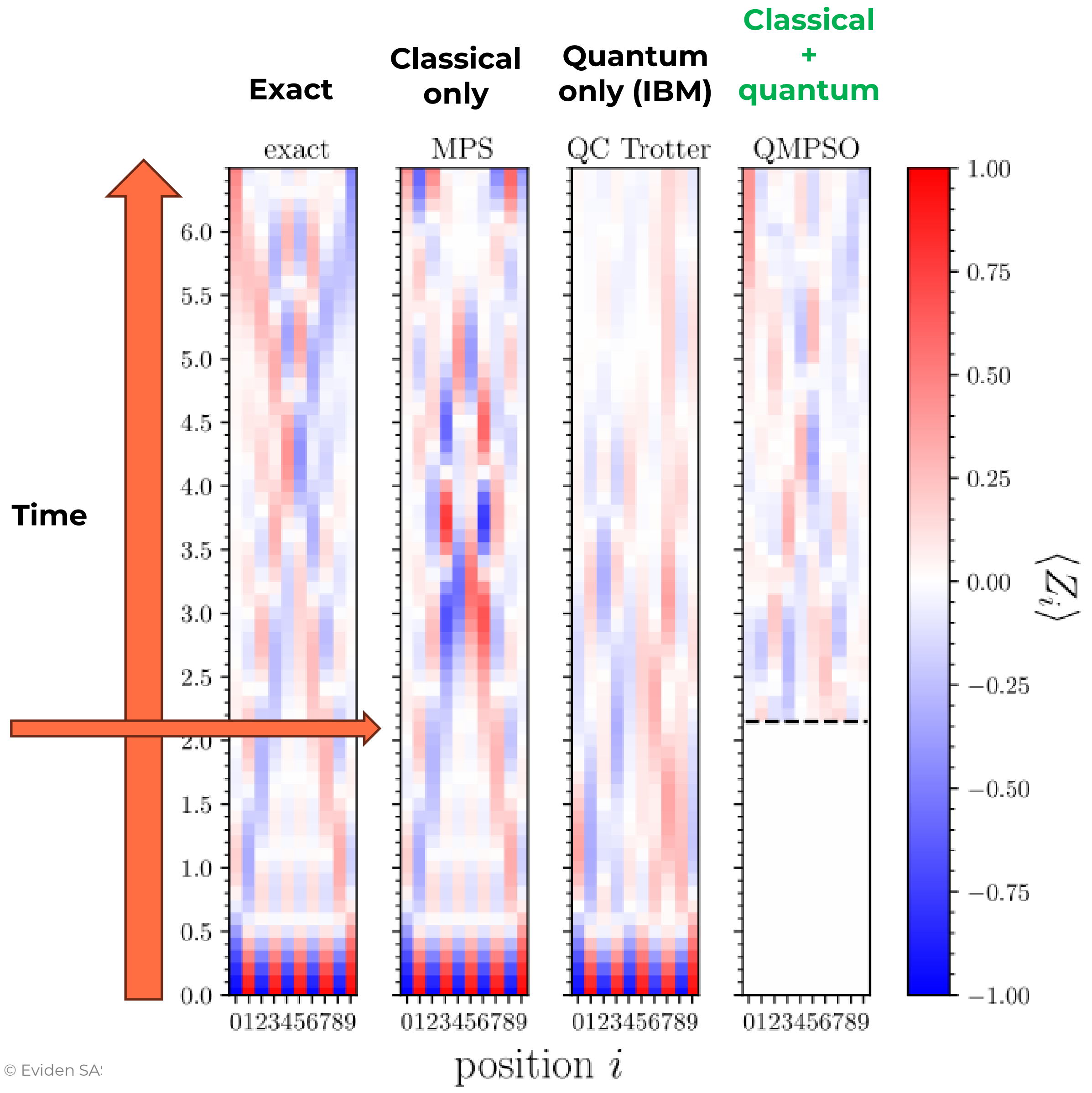

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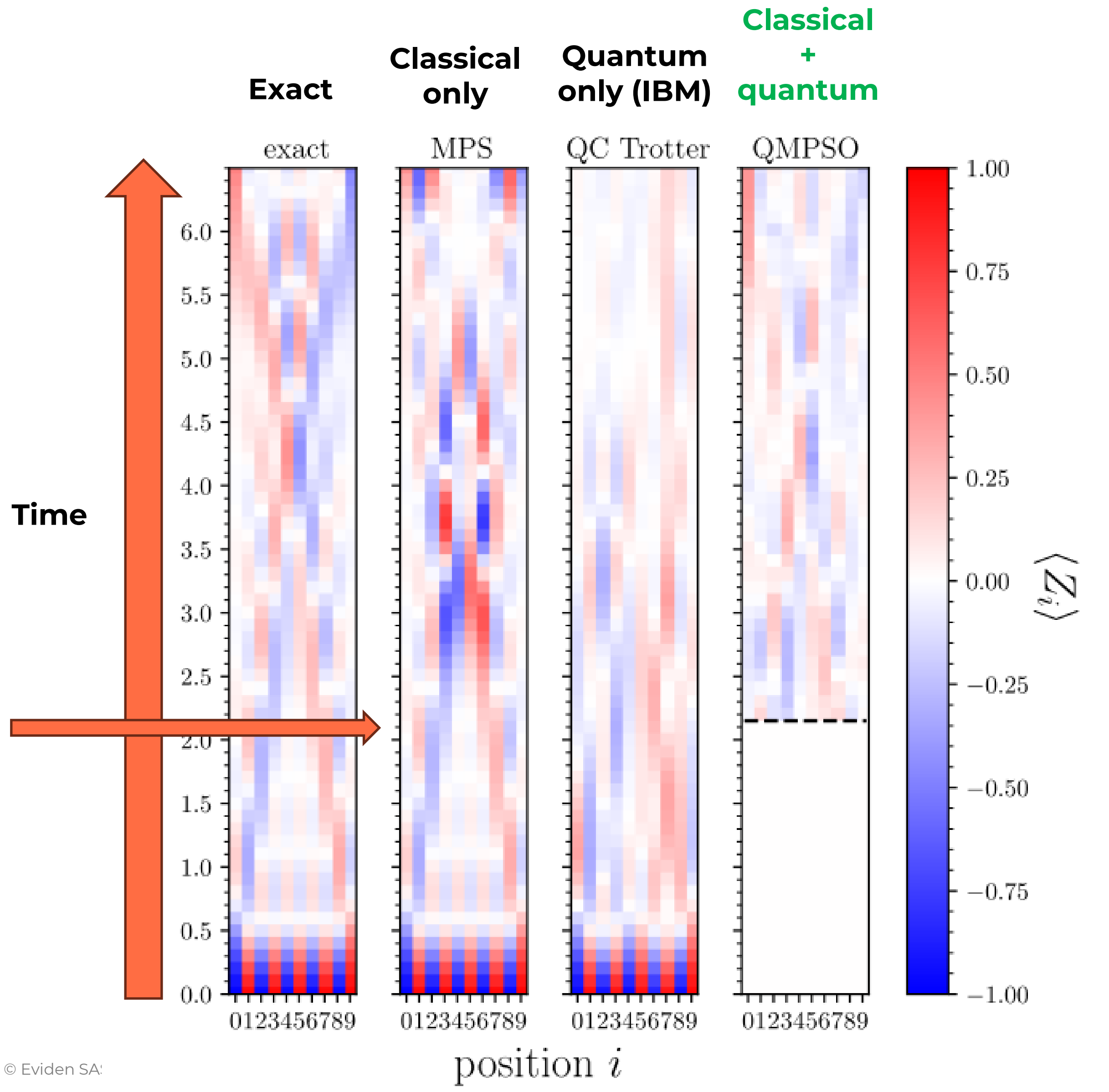
  $\Rightarrow$ max time to keep MPS ‘exact’
- Hybrid approach outperforms both others

Only proof of concept!

- **Artificially small RAM budget**: realistic budget would make it hard for QC to compete
- True challenge for TN: **2D (but same ideas apply)**



Conclusions of Part 3

Double role of tensor networks:

- Often the most advanced classical algorithm:
 a yardstick for quantum advantage
 (deflate quantum advantage claims)

- Can jump-start a quantum computation!
(Here, limited to 1D TN... true challenge: 2D)

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Not mentioned here… **a third role:**

- Tensor networks are also powerful tools to **emulate execution of quantum circuits**!

- Help interpret results of QCs with 100-1000 noisy qubits!

Key advantage: decoherence reduces entanglement S… and recall: $\chi \gtrsim 2^S$

$\Rightarrow$ Noisy QCs are easier for TNs!

$\Rightarrow$ **Eviden develops QC emulators with 100s qubits!**

See Müller, TA, Bertrand, 2403.00152

EVIDEN

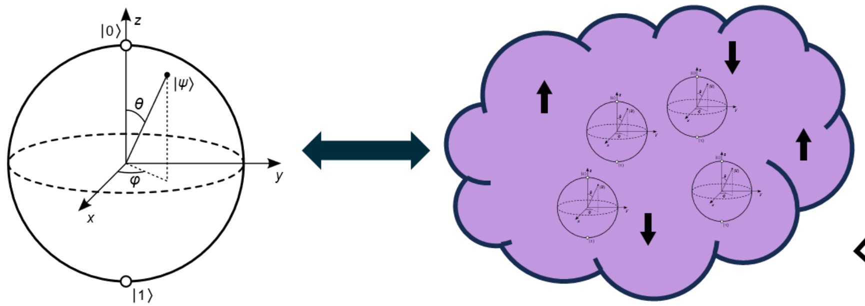
Outline

- Can we shorten circuits?
- Can we even avoid fermionic rules?
  Hubbard physics with Rydberg processors
- Hybridizing tensor networks and quantum algorithms
  Jump-starting quantum computations
- **Could we use quantum noise to our advantage?**

Can we use qubit noise to simulate a thermodynamical bath?

Bertrand, Besserve, Ferrero, TA, in preparation

Noisy quantum computer

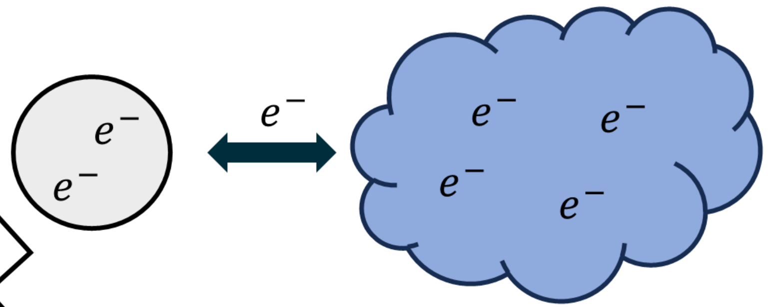


Dissipative processes:

- Amplitude damping → $S^{-} = |0\rangle\langle 1|$
- Dephasing → Z

formally the same

Many-body system + thermodynamic bath



Dissipative processes:

- Creation of particle → $c^{\dagger}$
- Annihilation of particle → c

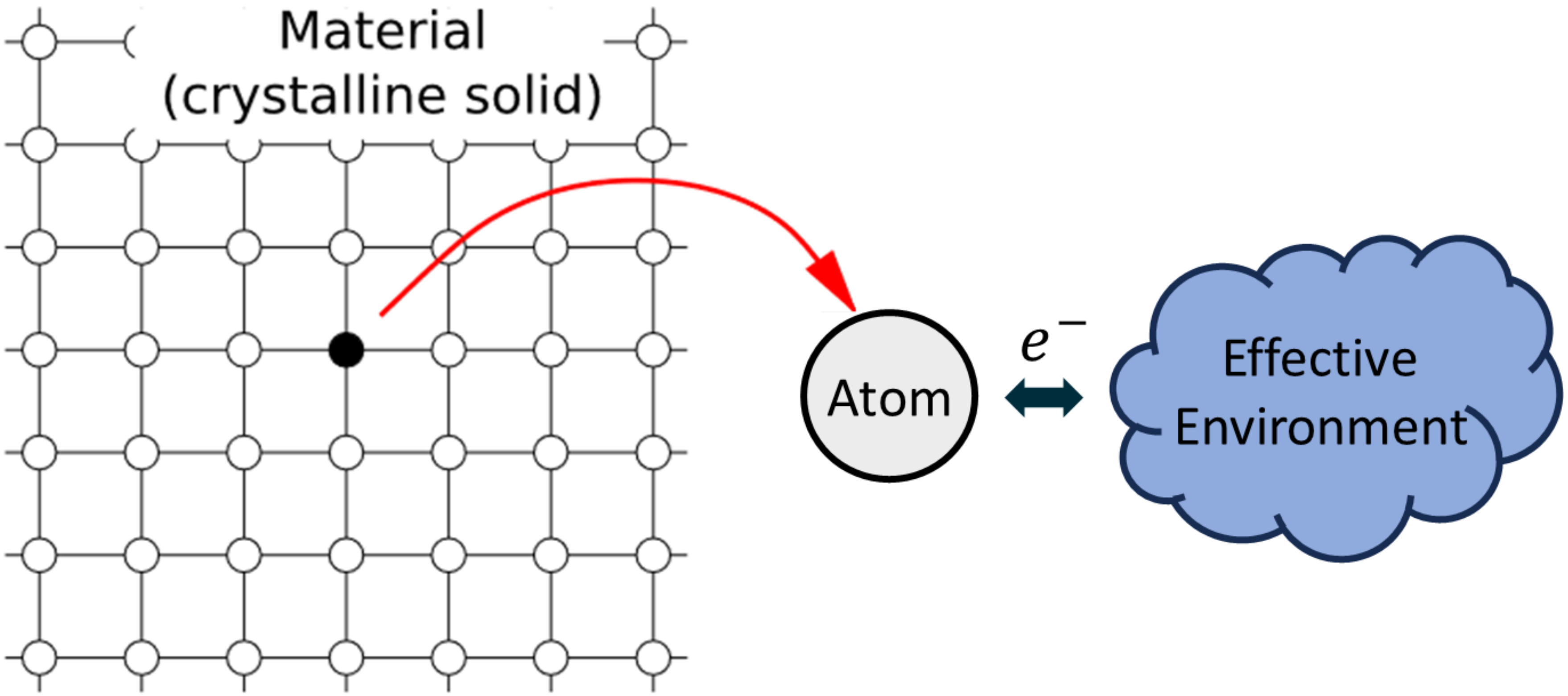
Slide courtesy of Corentin Bertrand

Dynamical mean field theory, an ideal playground

From a lattice problem to an atomic problem coupled to a bath

Bertrand, Besserve, Ferrero, TA, in preparation

e.g Hubbard model



Georges et al ‘96

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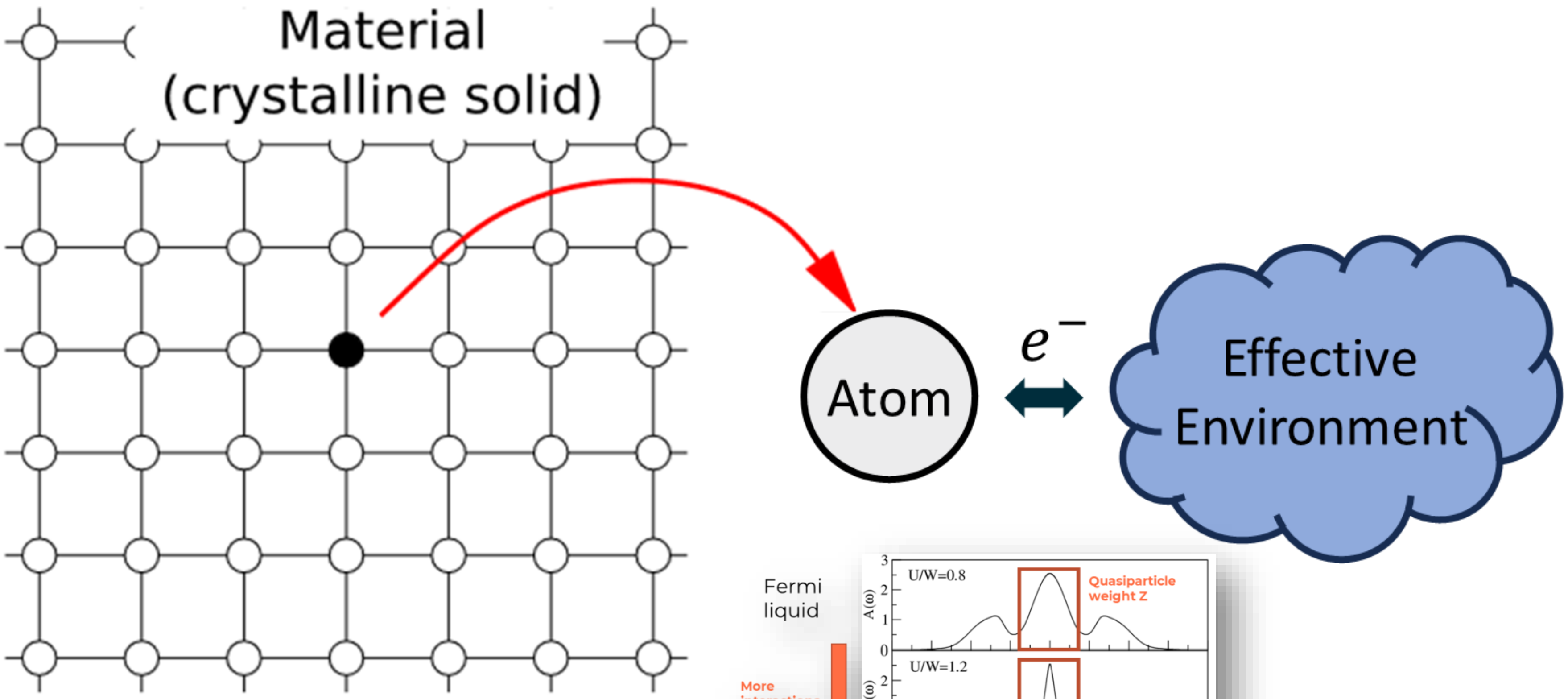
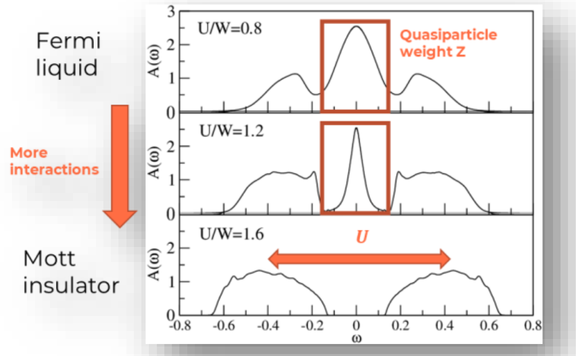




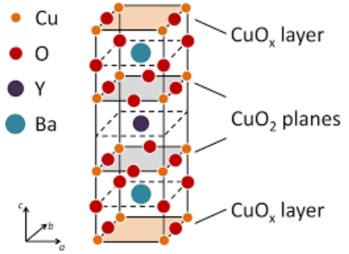
Georges et al ‘96

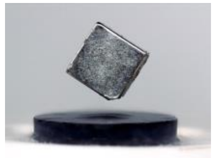
Slide courtesy of Corentin Bertrand

A workflow to leverage noisy qubits

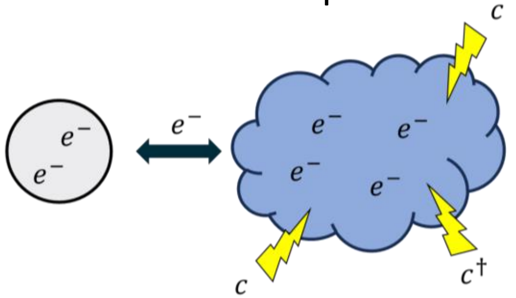
Bertrand, Besserve, Ferrero, TA, in preparation

Strongly correlated material





Fermionic impurity model with dissipation

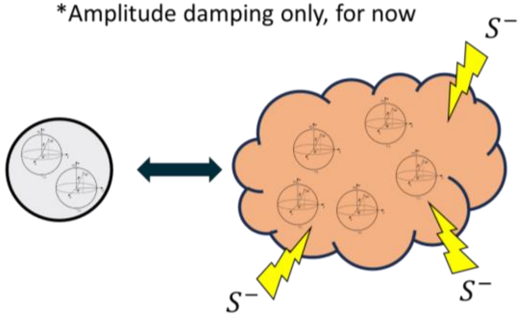


Arrigoni '13
Dorda '14 '15 '17
Schwarz '17

This work

Qubit model with noise*

*Amplitude damping only, for now



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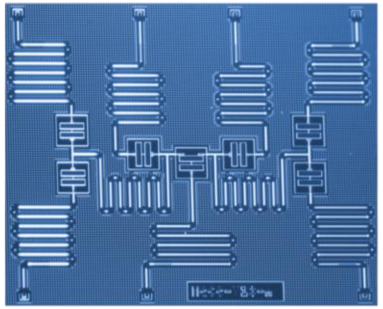
Simulate on noisy QC



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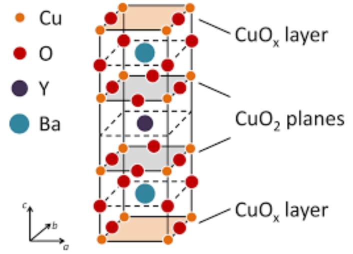

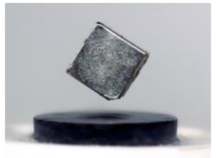

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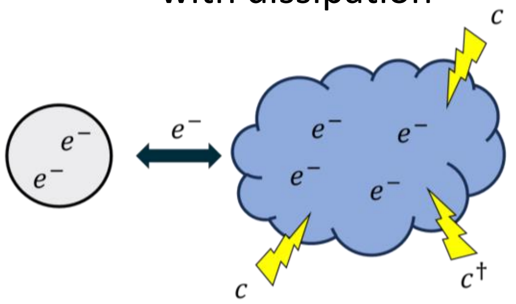

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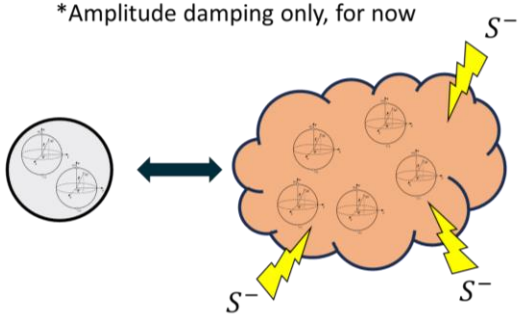

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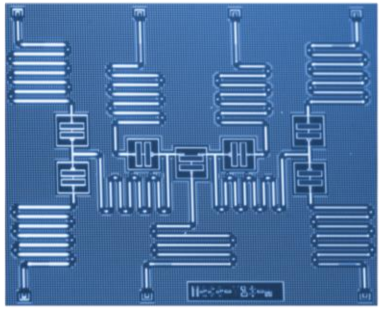

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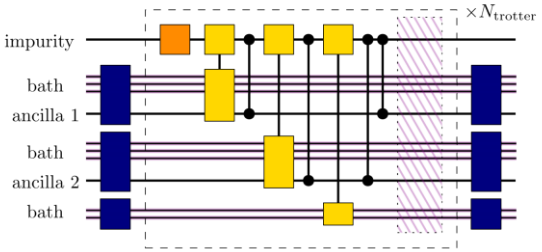

Slide courtesy of Corentin Bertrand

Bertrand, Besserve, Ferrero, TA, in preparation

What is the advantage of noise?

Coupling to a dissipative bath

- Alleviates **finite-size effects** (dissipation stems from large systems):

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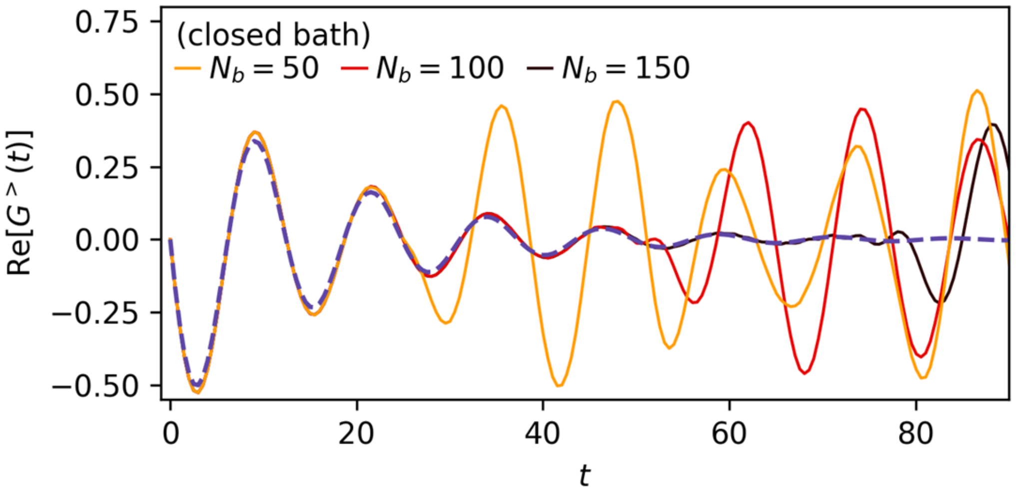

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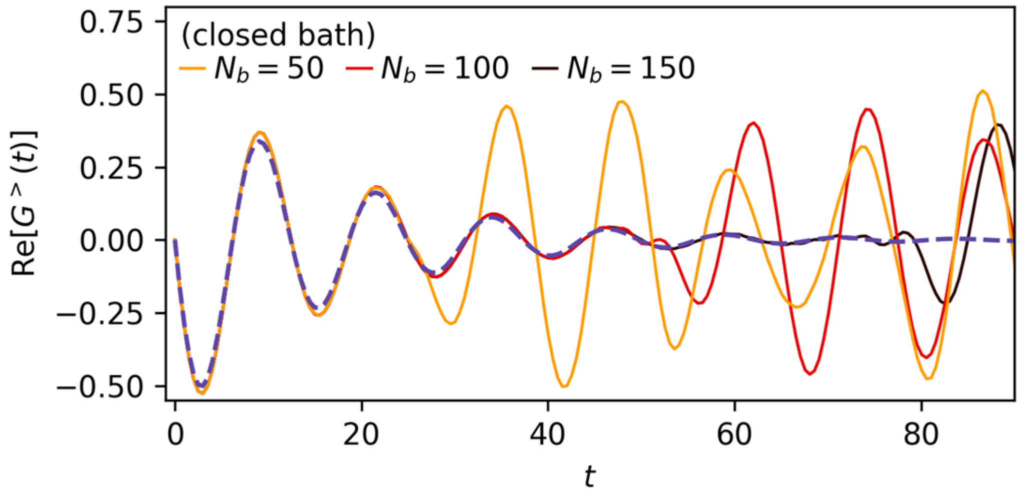

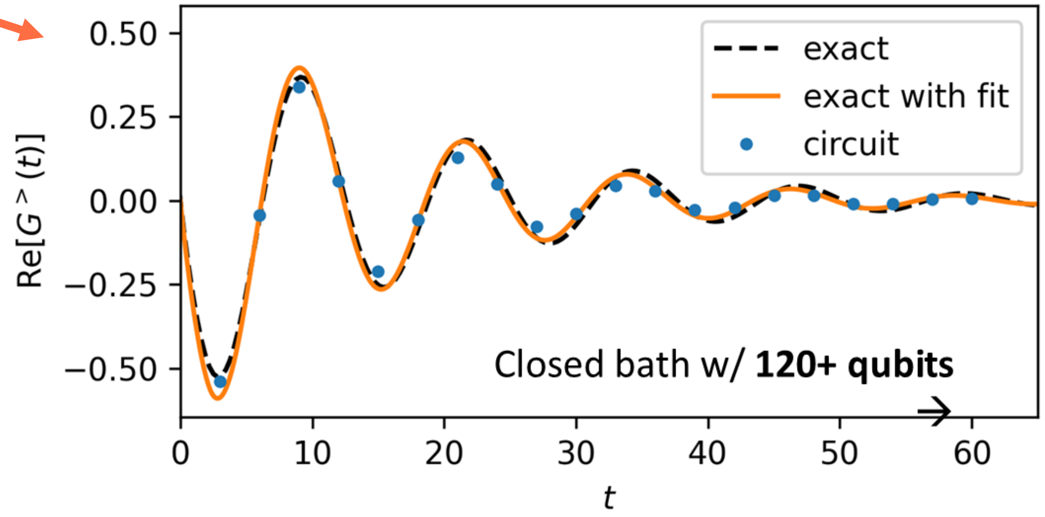

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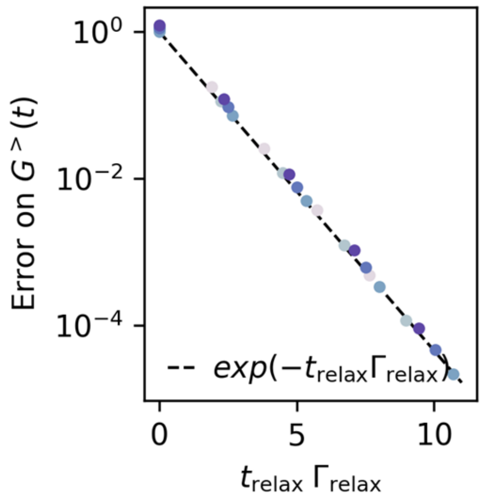
- **Speeds up state preparation** (dissipation helps reach steady state)



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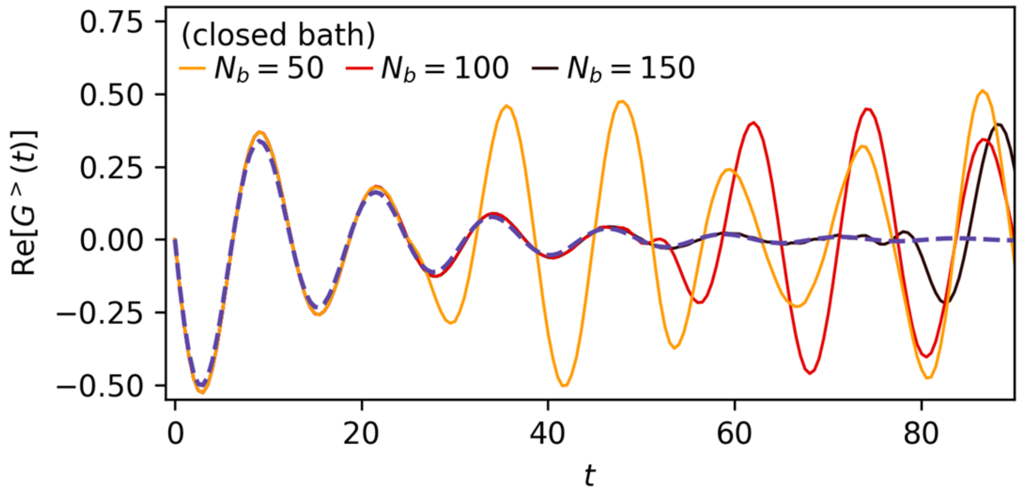

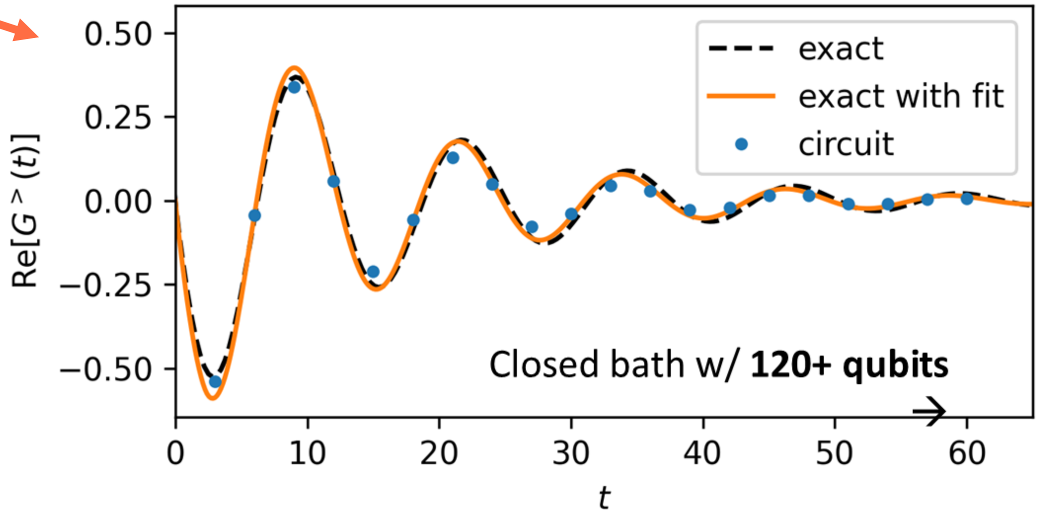

Conclusion

What prospects for today's processors?

Today, many-body platforms with **100-1000 particles/qubits**.

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Today's examples:

- Shorter circuit with natural orbitals
- Better convergence properties of PQE than VQE?
- Slave-spin to short-circuit fermionic overhead
- MPS to jump start QC
- Use noise to our advantage?

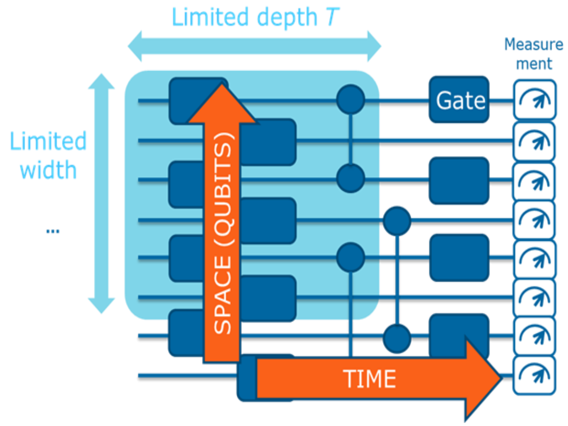
EVIDEN

Thanks

thomas.ayral@eviden.com

Known issues with the variational quantum eigensolver

Interesting variational circuits **are still too long!**



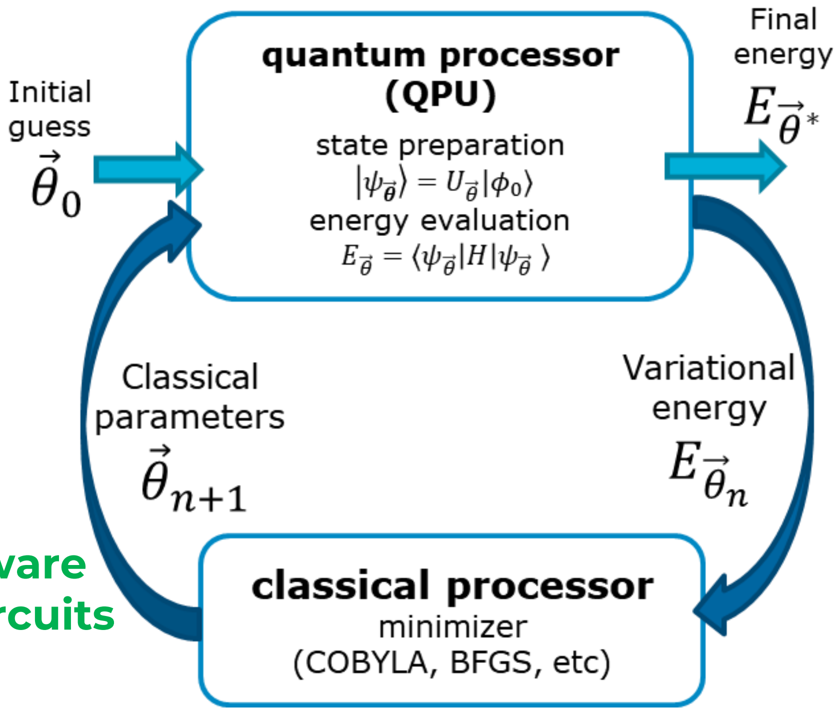
Noisy hardware... **Better hardware or shorter circuits**

Fermion antisymmetry:

$c_i^\dagger c_j$ leads to $X_i Z_{i+1} \dots Z_{j-1} X_j$

Hence longer circuits!

Better encodings or shortcut antisymmetry?



Is it hopeless?

Use QC for dynamics!

Measurement of $\langle\psi_\theta|H|\psi_\theta\rangle$:

statistical error $\Delta E \approx \frac{\|H\|_1}{\sqrt{N_{\text{samples}}}}$

Typically, $\|H\|_1 = 10$ Ha, $\Delta E = 1$mHa...

=> 10^8 samples / 10 kHz = 3 hours

(x number of optimization steps!)

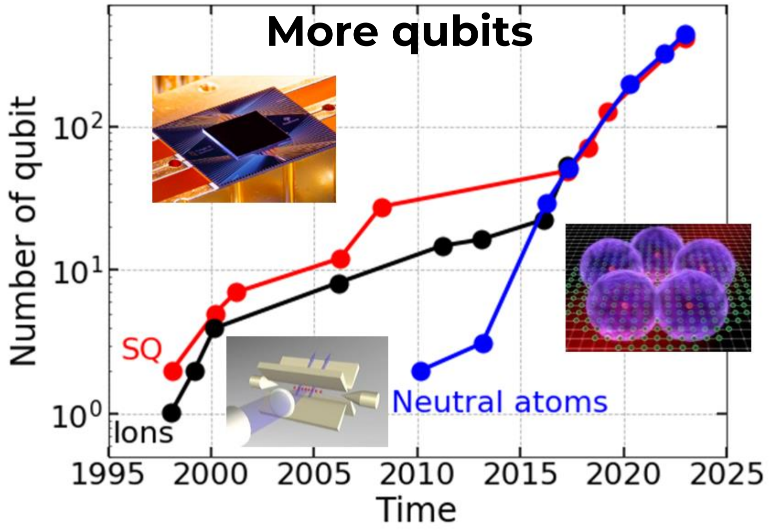
Don't measure $\langle\psi_\theta|H|\psi_\theta\rangle$, just sample!
Use VQE as input to LSQ algorithms

Barren plateau problem

Adaptive ansatz construction
Smarter initial starting point
Don't minimize $E(\theta)$
(find zero residues (cf coupled cluster), ...)

Should we directly turn to error-corrected QCs?

YES!



Courtesy of L.P Henry & L. Henriet @Pasqal

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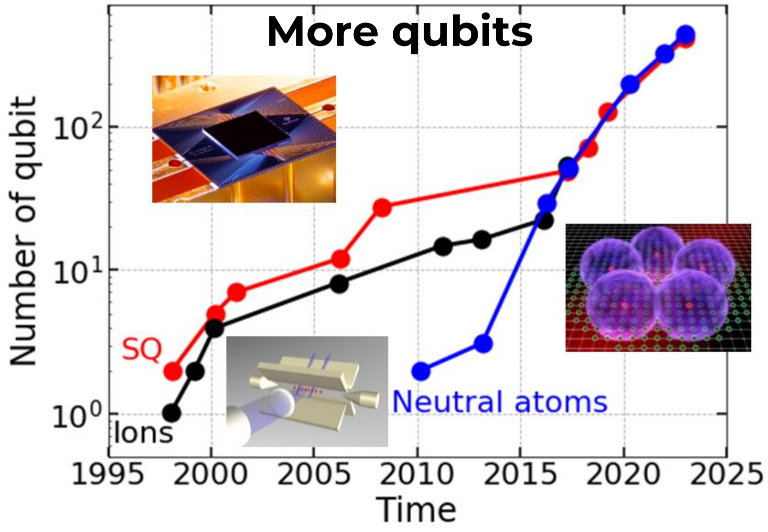

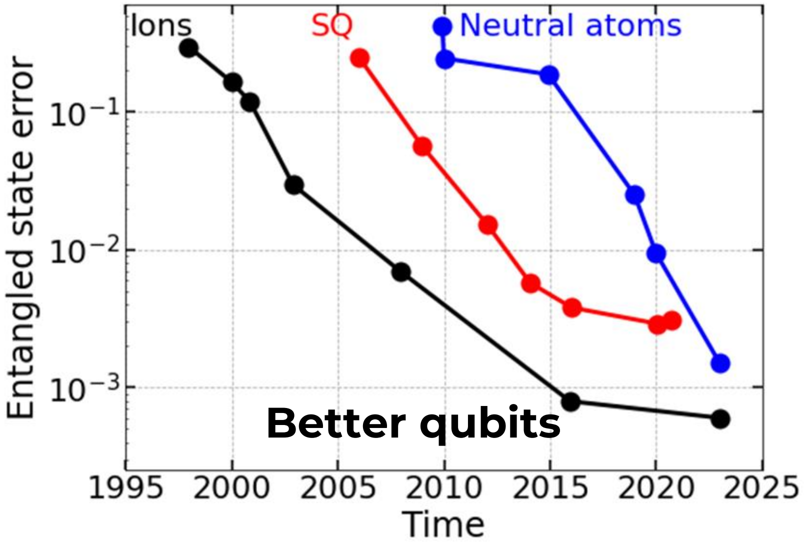

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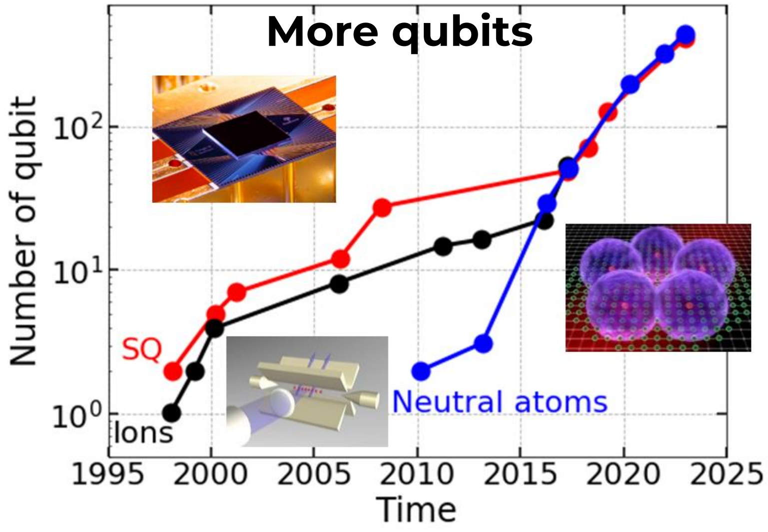
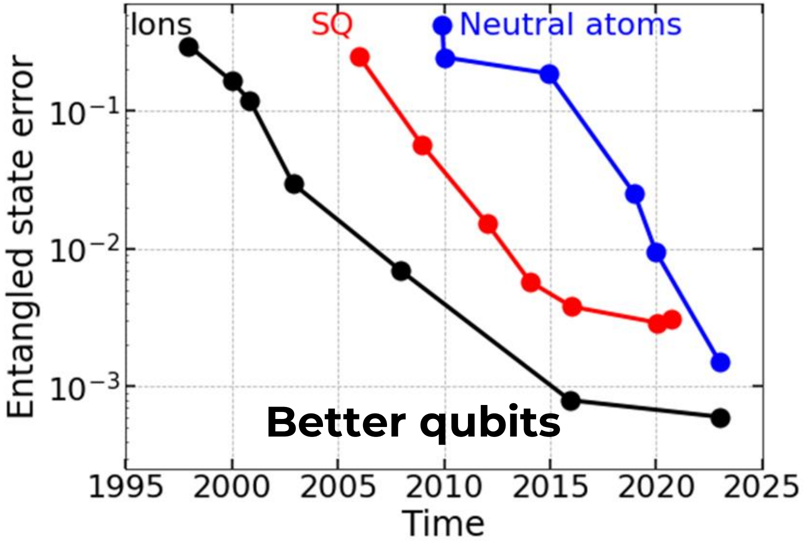
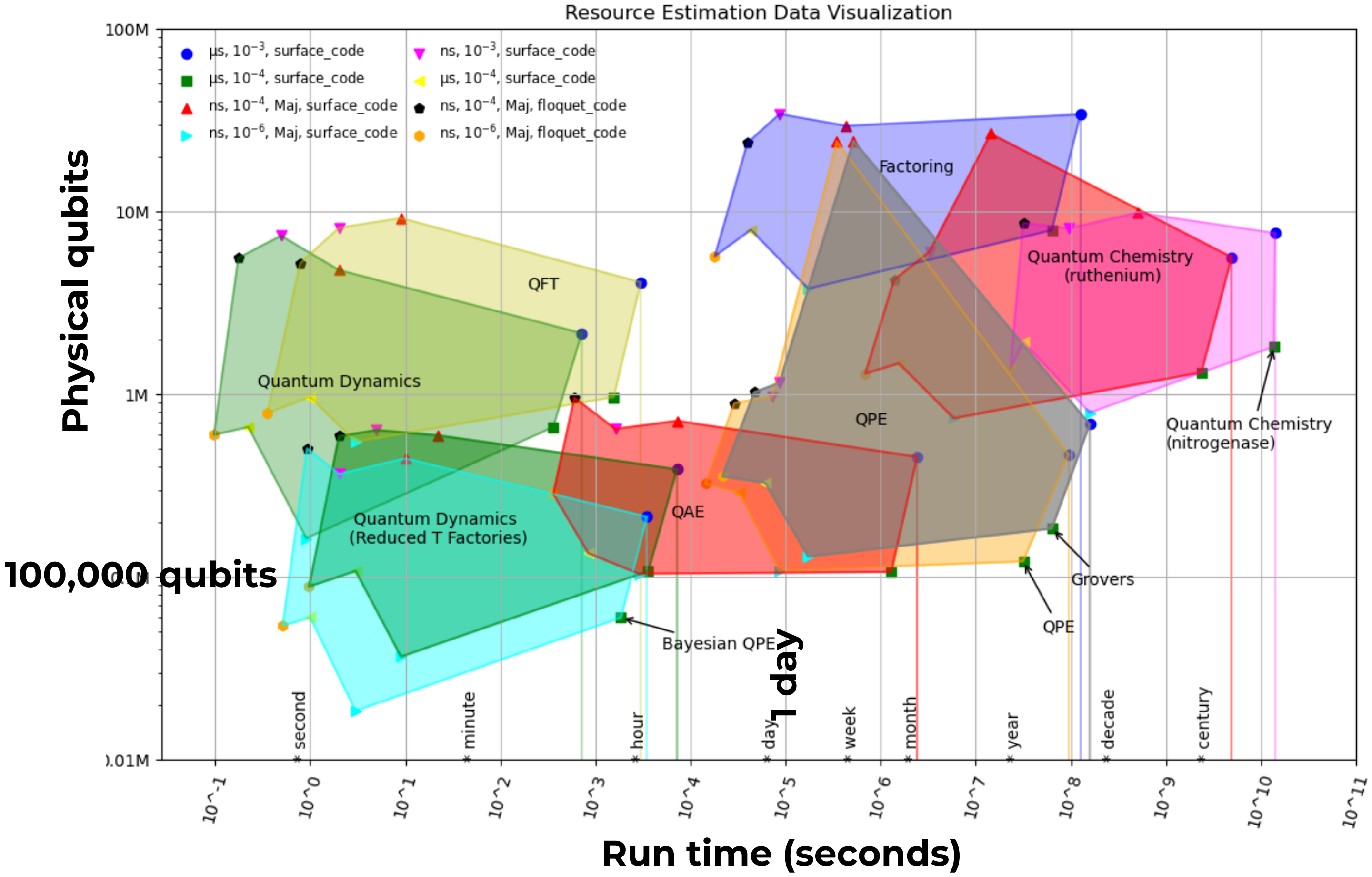




NO!



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GQI Quantum Resource Estimator Playbook
(Azure Quantum Resource Estimator)

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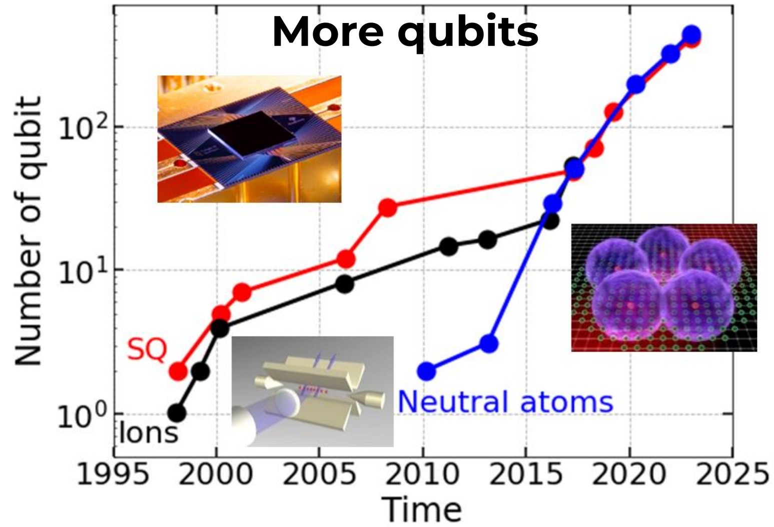

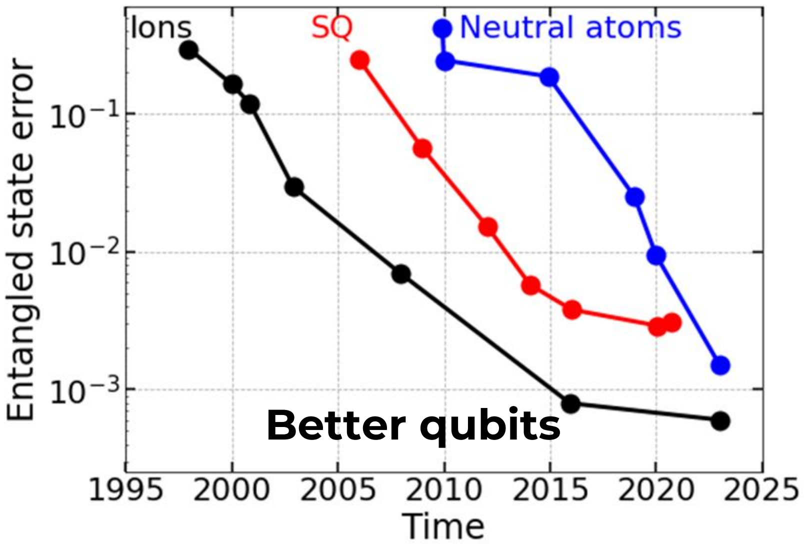

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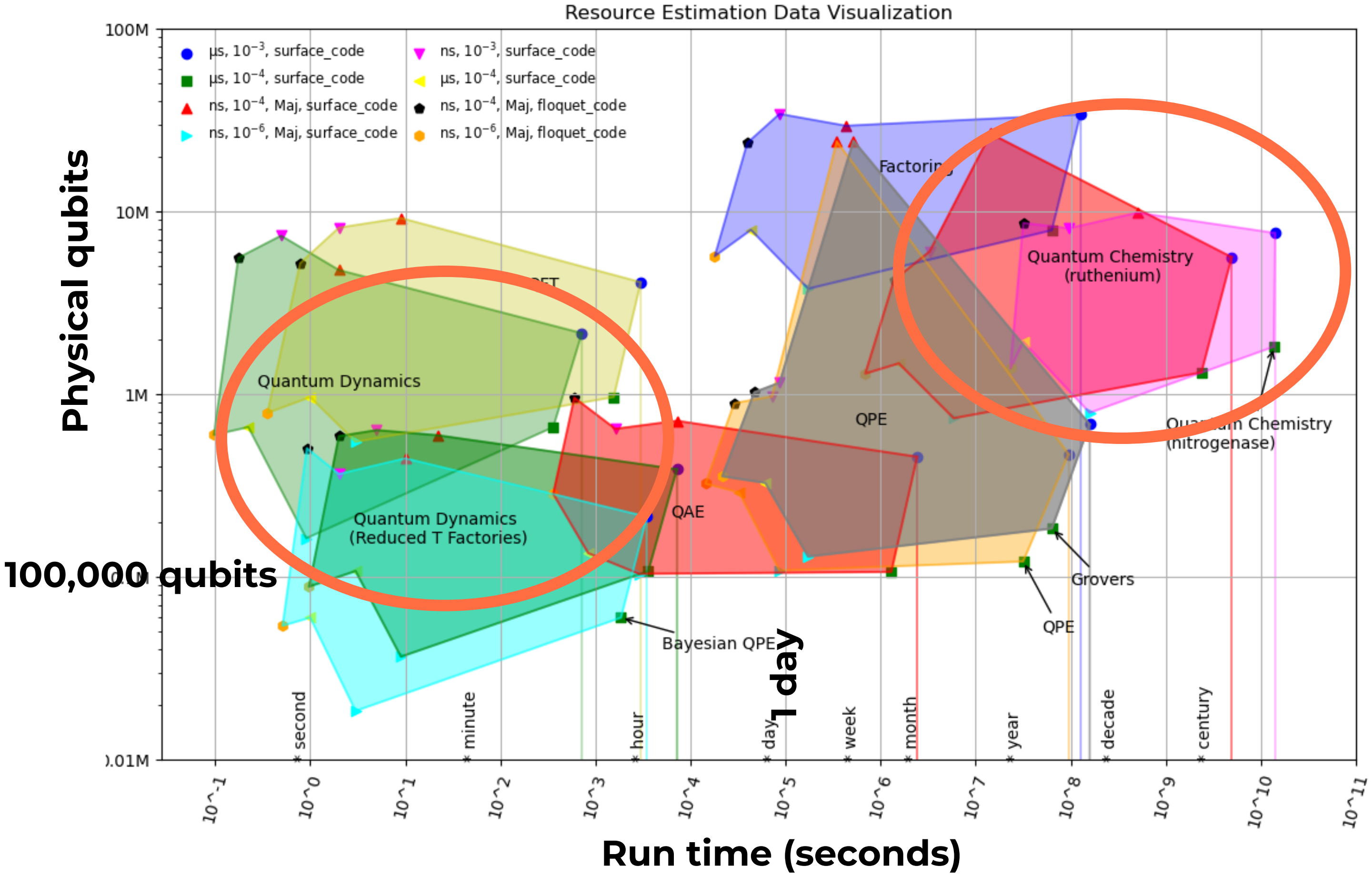

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Even if we had enough good qubits...

Louvet, TA, Waintal, 2306.02620

Orthogonality catastrophe in quantum phase estimation

QPE run time: $\propto 1/\Omega$

with Ω: overlap of input state with solution

Estimate of Ω:

$$\Omega \approx e^{-I_\Omega}$$

with

Energy error

$$I_\Omega = \frac{(E - E_0)^2}{2\sigma^2}$$

Variance

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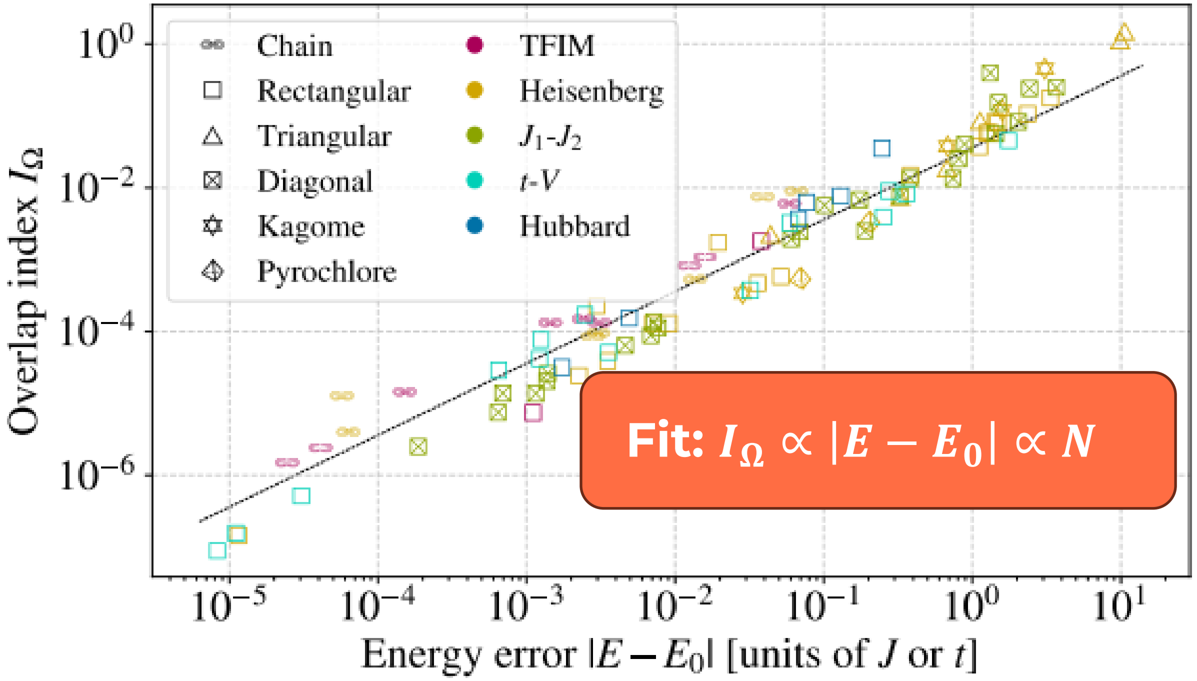
Test on state-of-the-art classical methods:



Fit: $I_\Omega \propto |E-E_0| \propto N$

Therefore: $\Omega \approx e^{-\alpha N}$

- Better inputs?
- Better phase estimation algorithms?