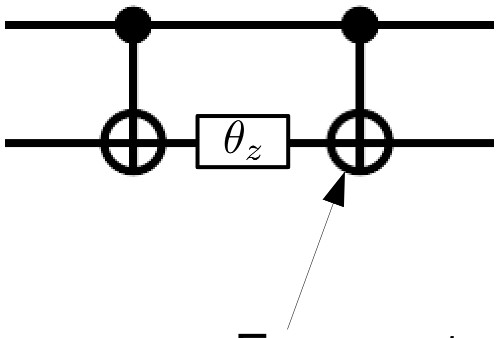
HQS QUANTUM SIMULATIONS

Can we find applications for quantum computers without quantum error correction?

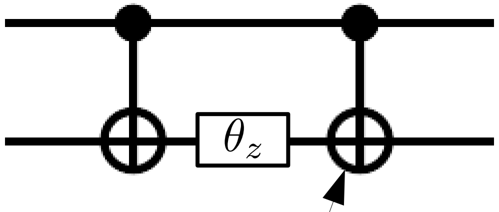
Michael Marthaler

NISQ computing: What should we expect?



Every gate has an error probability: ϵ

NISQ computing: What should we expect.



Every gate has an error probability: ϵ

Total number of gates: N_G

Number if Qubits: N_Q

Gate depth: D

Generally we want at least:

$$N_G < 1/\epsilon$$

For well parallelized algorithms

$$(N_G \approx N_Q D) \quad N_Q D < 1/\epsilon$$

One can often see that
what we really need is:

$$N_G \ll 1/\epsilon$$

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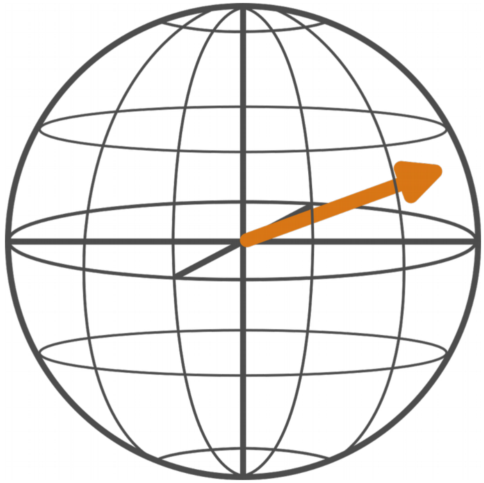
Agenda

1) Counting gates for quantum simulation

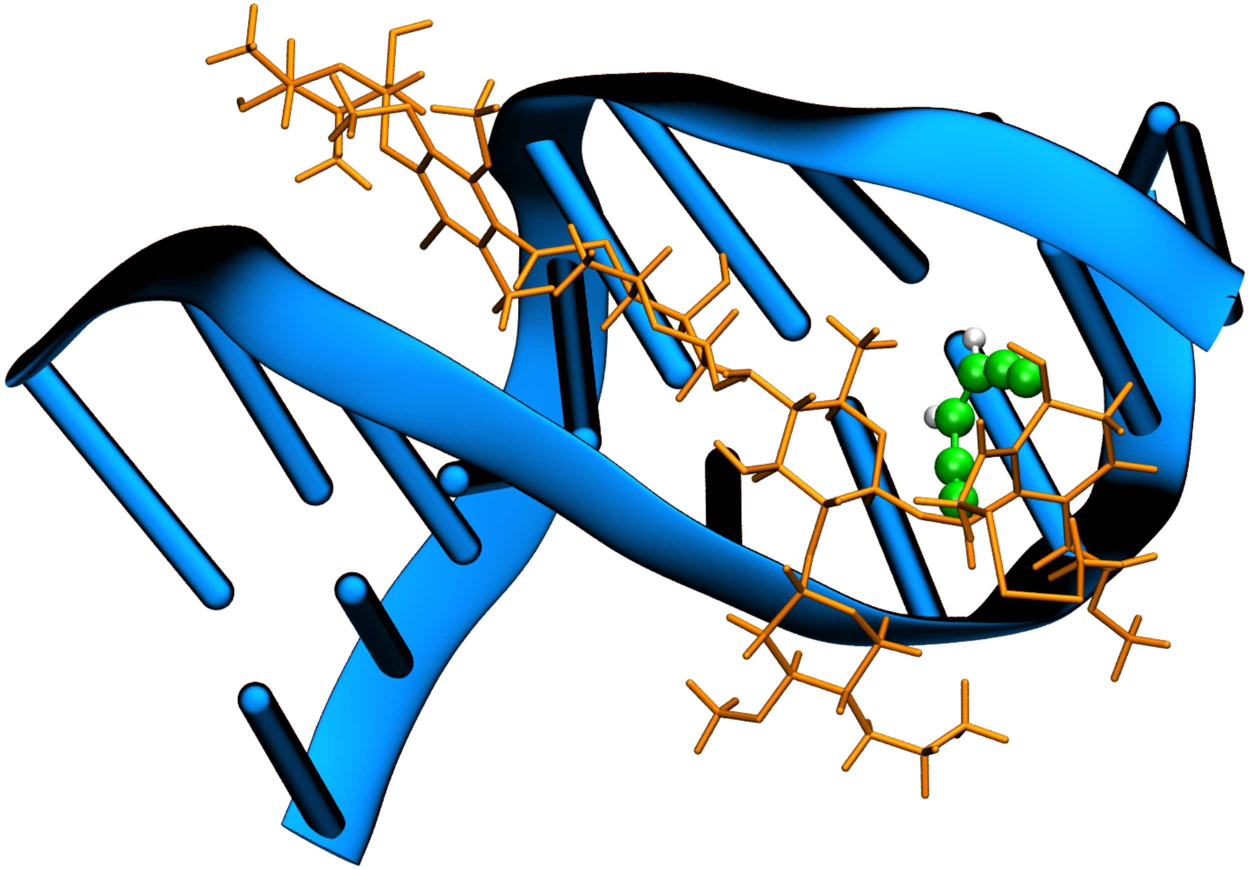
- General quantum chemistry $N_G \gg 1/\epsilon$
- Lattice models $N_G > 1/\epsilon$
- The optimal algorithm (on a 1D geometry) $N_G \propto N_Q D$

2) Quantum simulation: Total number of gates vs. depth, $N_G \ll 1/\epsilon$ or $D \ll 1/\epsilon$

3) Noise in quantum simulation: From $\ll$ to $<$



Counting gates for quantum simulation



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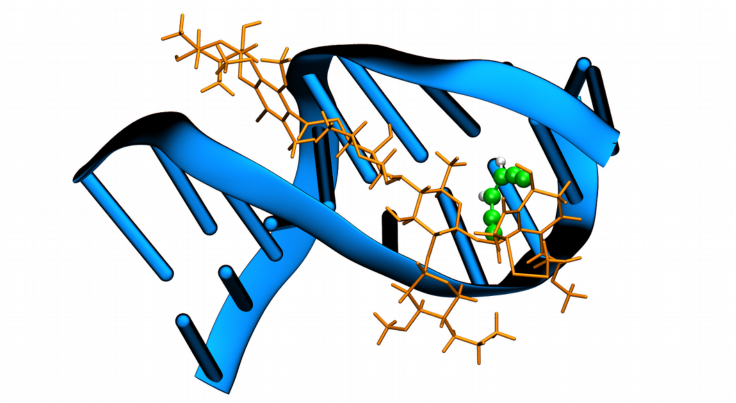
The Hamiltonian

Simulating the dynamics of a molecule or solid.



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

The full Hamiltonian in the active space for N orbitals.

Number of terms: N^4

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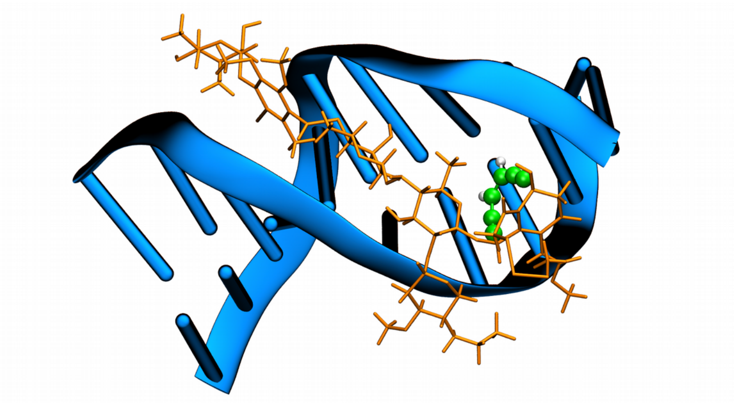
Trotter expansion

Simulating the dynamics of a molecule or solid.



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

Time evolution: $$U(T) = \left(e^{-iH_S\, T/m}\right)^m \approx \left(\prod_n e^{-iH_n \tau}\right)^m \qquad \tau = \frac{T}{m}$$

We assume that a unitary operator similar to a time evolution can prepare the ground state.

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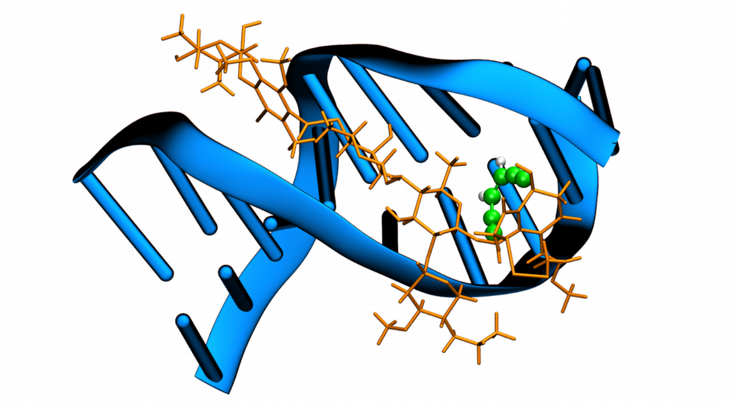
Trotter expansion

Simulating the dynamics of a molecule or solid.



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Time evolution: $U(T) = \left(e^{-iH_S T/m}\right)^m \approx \left(\prod_n e^{-iH_n \tau}\right)^m \quad \tau = \frac{T}{m}$

Number of terms: N^4

Number of gates $N_G \propto N^4$ with a modest constant factor.

Quantum advantage at $N \approx 50 \Rightarrow N_G > 625 \times 10^4$

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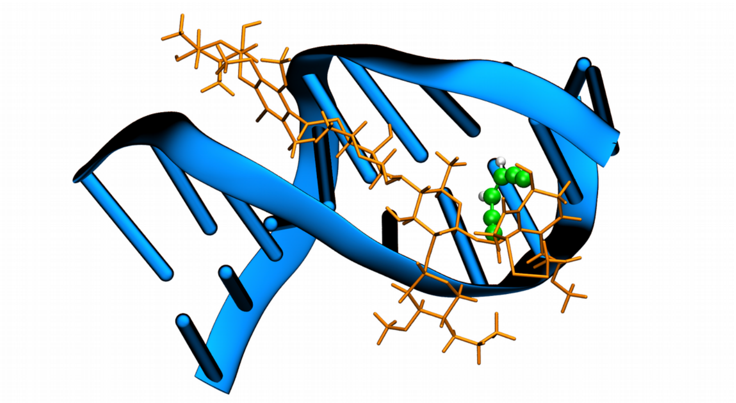
Gate count for full quantum chemistry

Simulating the dynamics of a molecule or solid.



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

Time evolution: $U(T) = \left(e^{-iH_S T/m}\right)^m \approx \left(\prod_n e^{-iH_n \tau}\right)^m \quad \tau = \frac{T}{m}$

Number of terms can be reduced to : N^3 M. Motta, E. Ye, J. R. McClean, Z. Li, A. J. Minnich, R. Babbush, G. Kin-Lic Chan, arxiv:1808.02625

Number of gates $N_G \propto N^3$ with a modest constant factor.

Quantum advantage at $N \approx 50 \Rightarrow N_G > 125 \times 10^3$

For any existing device we see: $N_G \gg 1/\epsilon$

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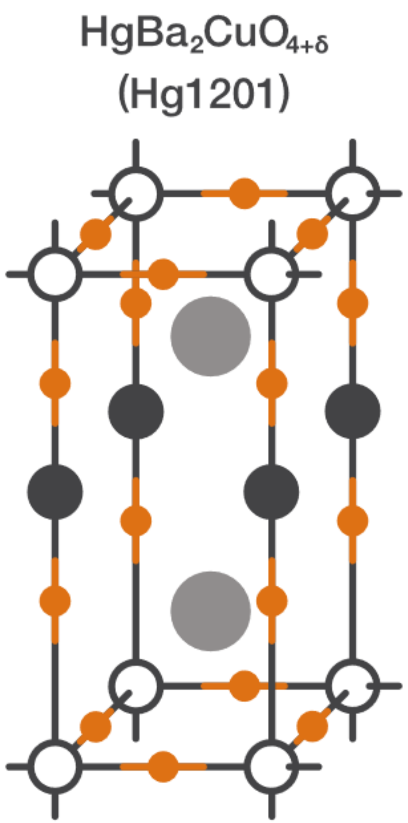
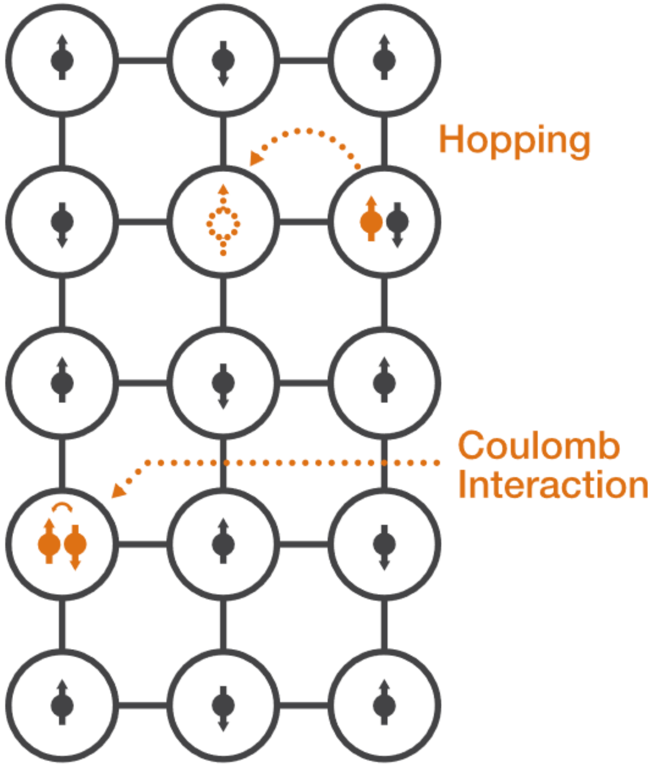
Lattice models



High-T_c superconductor



Hubbard Model

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Lattice models: simplified Hamiltonian

Full quantum chemistry:

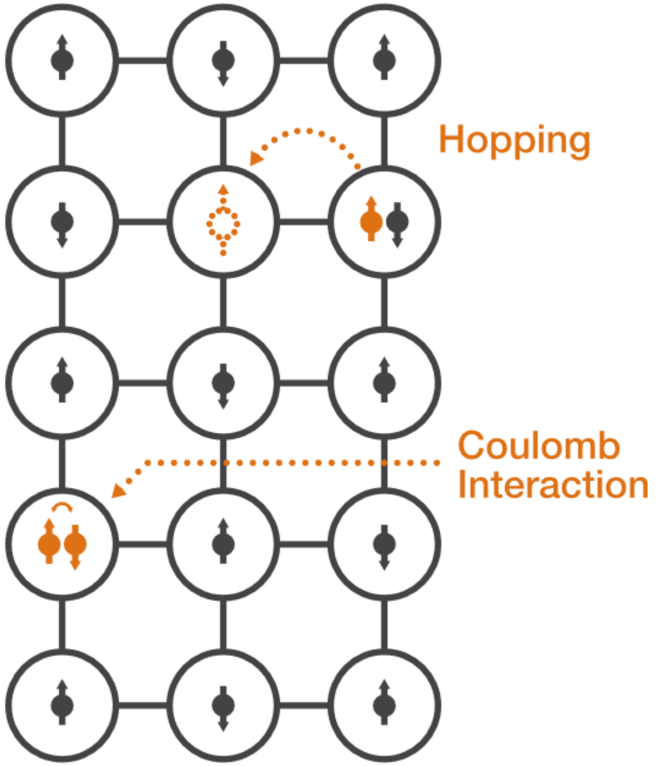
$$H_S = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} v_{ijkl} c_i^\dagger c_k^\dagger c_l c_j$$

Trotter step with at least order N^3 gates

Lattice model:

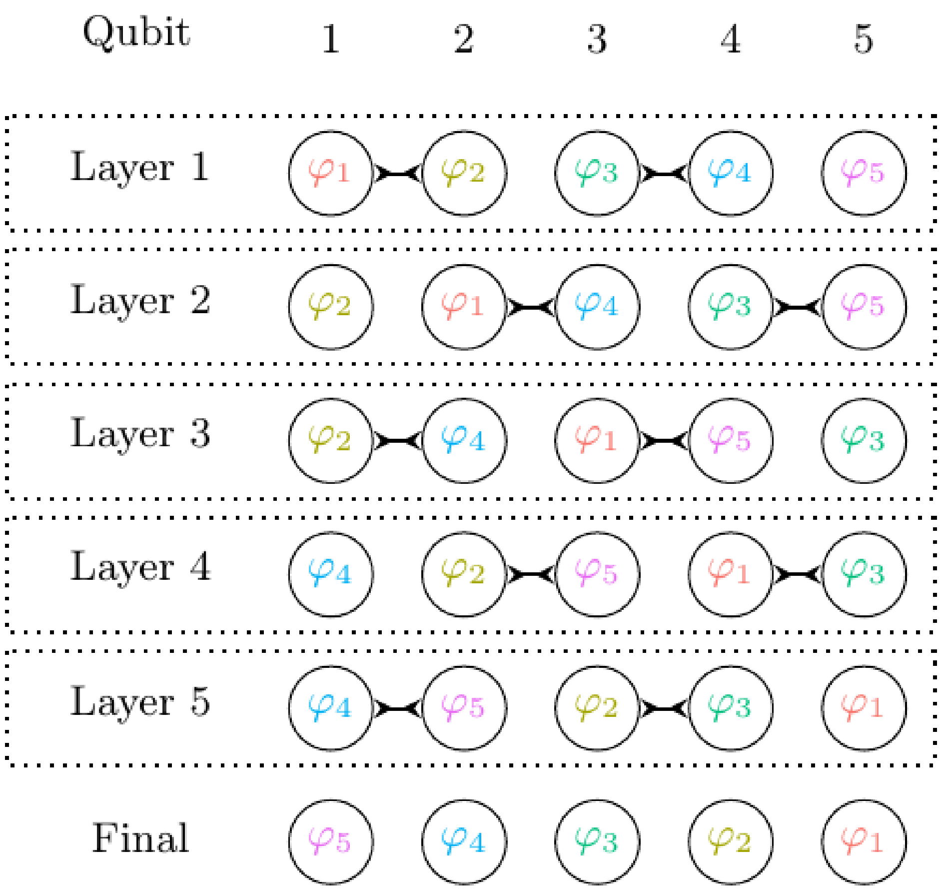
$$H_S = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ij} U_{ij} c_i^\dagger c_i c_j^\dagger c_j$$

Trotter step with order N^2 gates



Hubbard Model

Optimal algorithm on a 1D geometry



Ian D. Kivlichan, Jarrod McClean, Nathan Wiebe, Craig Gidney, Alán Aspuru-Guzik, Garnet Kin-Lic Chan, Ryan Babbush, Phys. Rev. Lett. 120, 110501 (2018)

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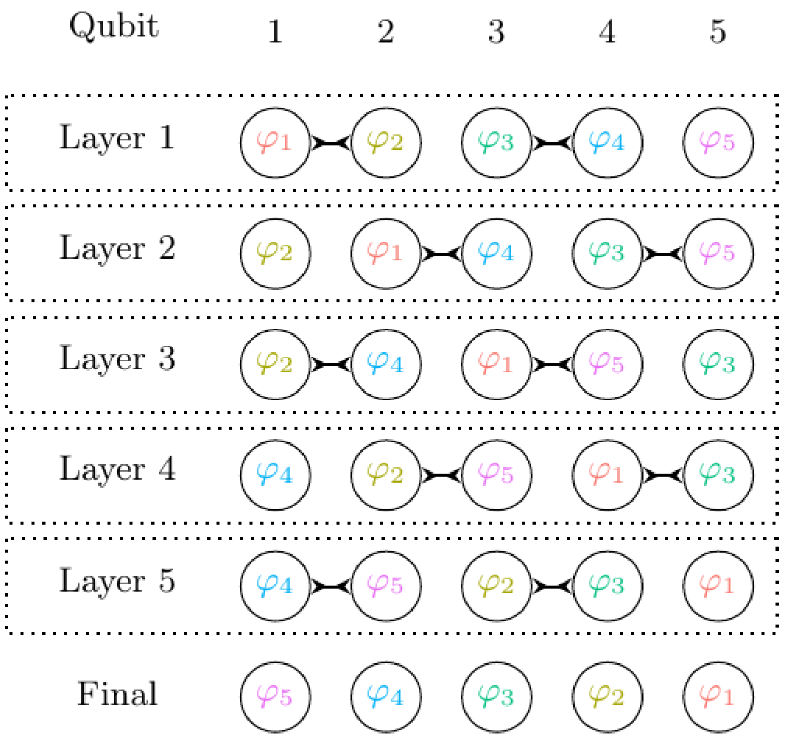
Optimal algorithm for lattice models

$$H_S = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ij} U_{ij} c_i^\dagger c_i c_j^\dagger c_j \qquad U(t) = \left(e^{-iH_S t/m}\right)^m$$

Using SWAP (or fSWAP) we can simulate lattice system on a 1D geometry with a very small gate depth depth.

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

Gate depth per Trotter-step: N



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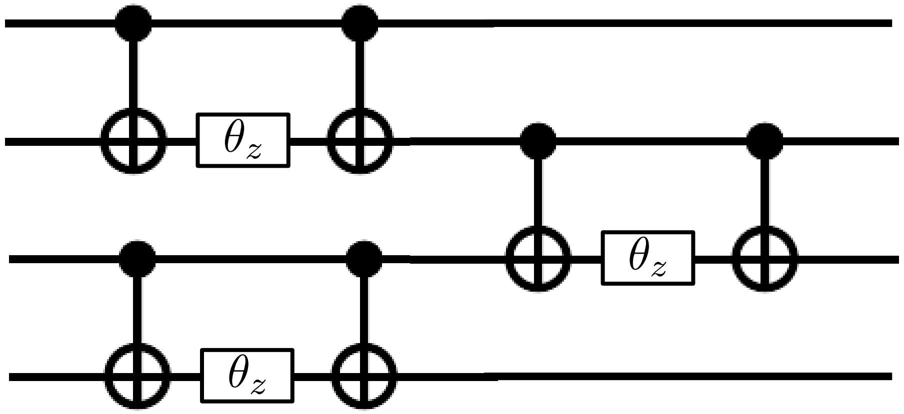
Quantum simulation: Total number of gates vs. depth



Depth: 6

Total number of gates: 9

Depth corresponds to the time you need to run an algorithm.

Quantum simulation: depth or total number?

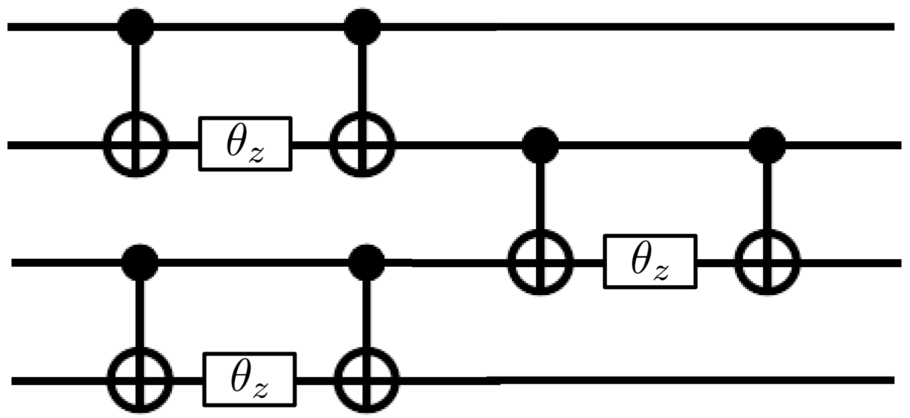
Time evolution of the noisy quantum computer:

$$U = e^{i \int_0^t dt (H_{\mathrm{qc}}(t) + H_\gamma)}$$

Hamiltonian we want to simulate:

$$H_S = \sum_n H_n$$

We will use the sum for the Trotter expansion



QUANTUM SIMULATIONS

The noise quantum computer

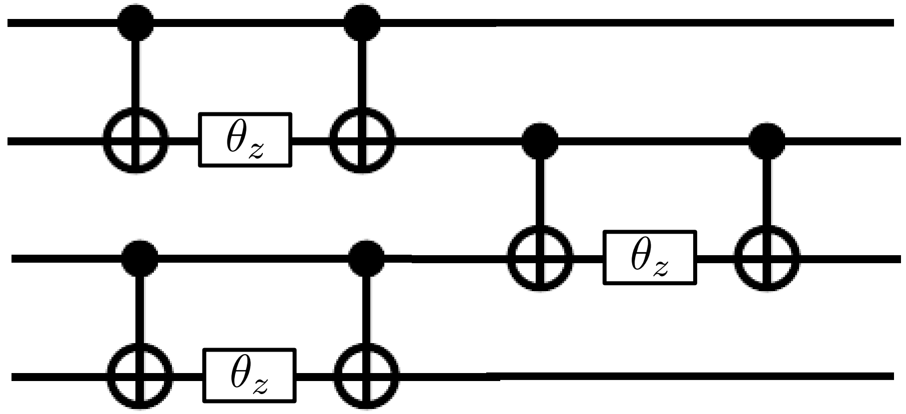
Time evolution of the noisy quantum computer:

$$U = e^{i \int_0^t dt (H_{\mathrm{qc}}(t) + H_\gamma)}$$

$t =$ time to implement a Trotter step

Hamiltonian we want to simulate:

$$H_S = \sum_{n=1}^{M} H_n$$



The quantum computer performing a simulation without noise:

$$U = e^{i \int_0^t dt H_{\mathrm{qc}}(t)} = \Pi_n e^{i H_n \frac{t}{M}} \approx e^{i H_S \tau} \qquad \tau = t/M$$

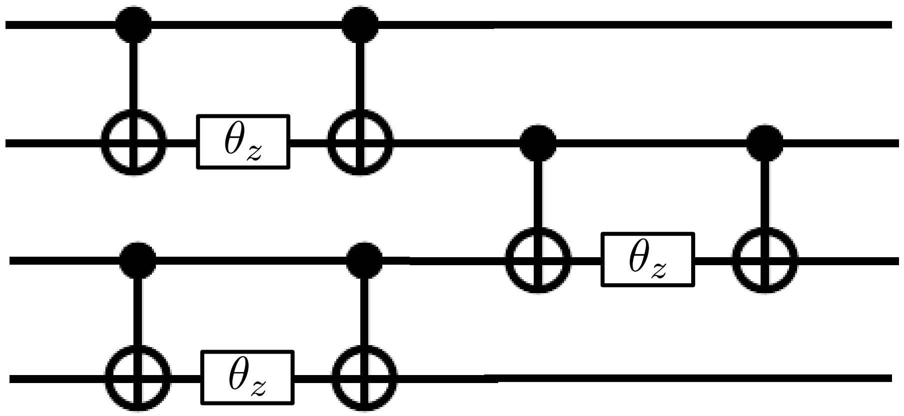
Quantum Simulation: Total number of gates vs. depth

Time evolution of the noisy quantum computer:

$$U = e^{i\int_0^t dt(H_{\mathrm{qc}}(t)+H_\gamma)}$$

Hamiltonian we want to simulate:

$$H_S = \sum_{n=1}^{M} H_n$$



The quantum computer performing a simulation with noise:

$$U = e^{i\int_0^t dt\,(H_{\mathrm{qc}}(t)+H_\gamma)} = \Pi_n e^{iH_n\,t/M+iH_\gamma\,t/M} \approx e^{iH_S\tau+iMH_\gamma\tau} \qquad \tau = t/M$$

We make here a simple assumption about the time needed to create $e^{iH_n\tau}$

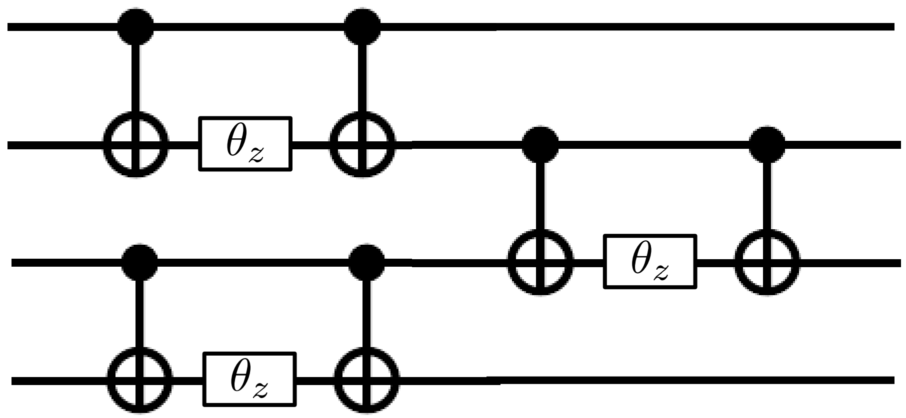
Quantum Simulation: Total number of gates vs. depth

Time evolution of the noisy quantum computer:

$$U = e^{i\int_0^t dt(H_{\mathrm{qc}}(t)+H_\gamma)}$$

Hamiltonian we want to simulate:

$$H_S = \sum_{n=1}^{M} H_n$$



The quantum computer performing a simulation with noise:

$$U = e^{i\int_0^t dt\,(H_{\mathrm{qc}}(t)+H_\gamma)} = \Pi_n e^{iH_n\frac{t}{M}+iH_\gamma\frac{t}{M}} \approx e^{iH_S\tau+iMH_\gamma\tau} \qquad \tau = t/M$$

Within our simplification $M = D$

Even if we exactly keep track of all number of gate and gate times:
Strength of noise scales with Depth!

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Example

Hamiltonian we want to simulate:

$$H_S = \frac{1}{2}\epsilon_1\sigma_z^1 + \frac{1}{2}\epsilon_2\sigma_z^2 + \frac{1}{2}\epsilon_3\sigma_z^3 + g_1\sigma_x^1\sigma_x^2 + g_2\sigma_x^2\sigma_x^3 = H_1 + H_2 + H_3$$

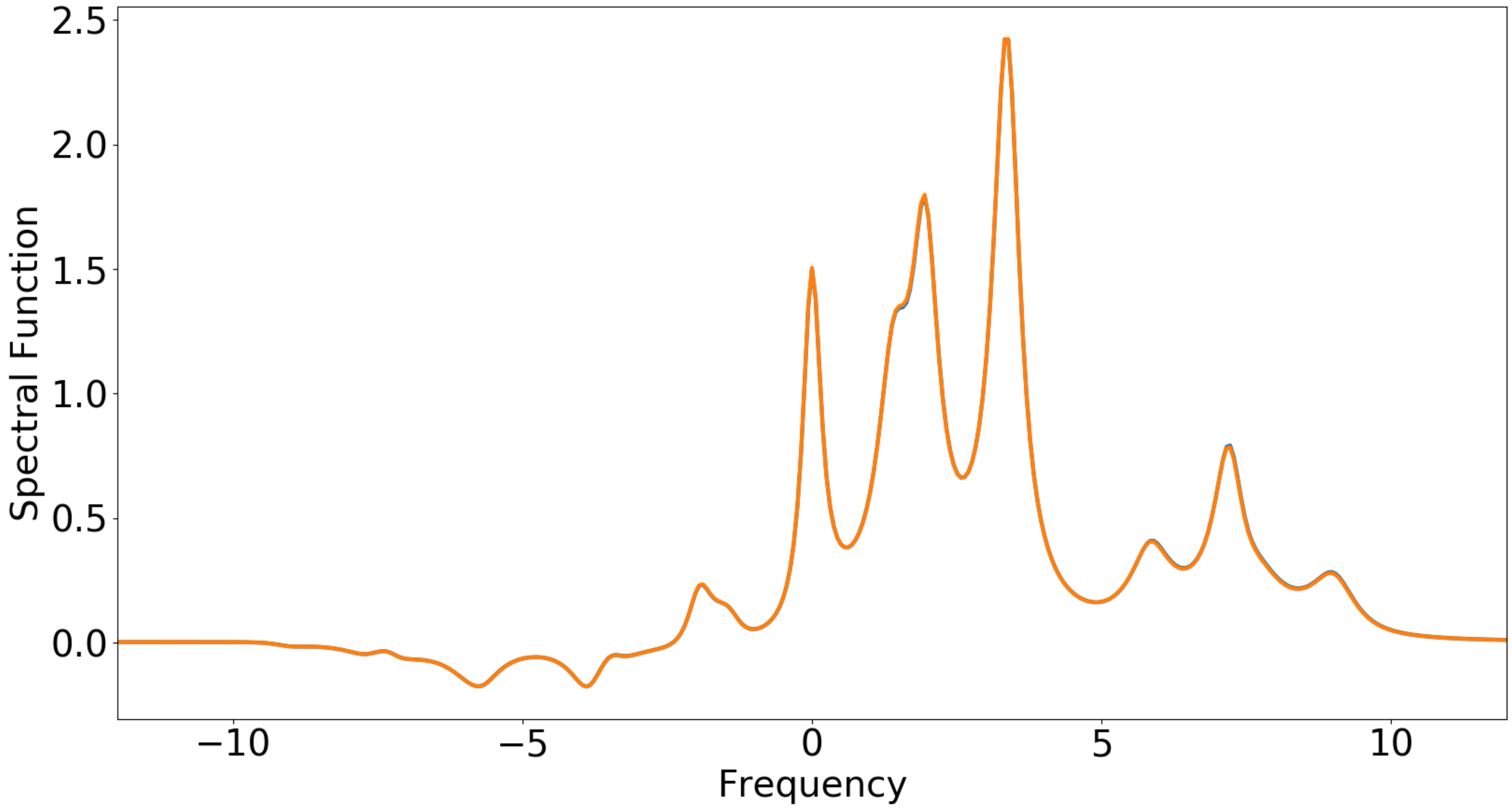
$$H_1 = \frac{1}{2}\epsilon_1\sigma_z^1 + \frac{1}{2}\epsilon_2\sigma_z^2 + \frac{1}{2}\epsilon_3\sigma_z^3 \qquad H_2 = g_1\sigma_x^1\sigma_x^2 \qquad H_3 = g_2\sigma_x^2\sigma_x^3$$

The quantum computer performing a simulation with noise:

$$U = e^{i\int_0^t dt(H_{\mathrm{qc}}(t)+H_\gamma)} = \Pi_{n=1}^3 e^{iH_n\frac{t}{n}+iH_\gamma\frac{t}{n}} \approx e^{iH_S\tau+i3H_\gamma\tau} \qquad \tau = t/3$$

Example

Simulation of five qubits: Comparing Trotterized to effective master equation simulation.



Our effective model fits the noisy gate based simulation exactly.

Quantum Simulation: Total number of gates vs. depth

Time evolution of the noisy quantum computer:

$$U = e^{i \int_0^t dt (H_{\mathrm{qc}}(t) + H_\gamma)}$$

Simulation with noise:

$$U = e^{i H_S \tau + i \alpha H_\gamma \tau}$$

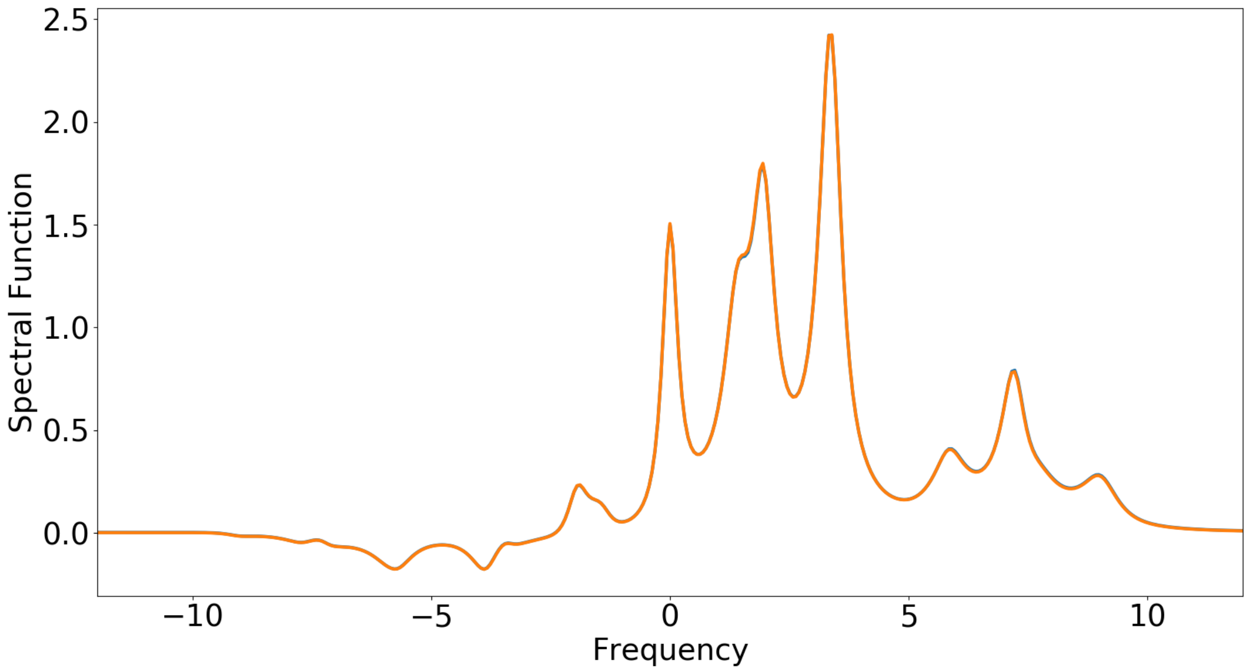
Scaling factor:

$$\alpha = D \frac{\tau_G}{\tau}$$

Actual time per gate

Hamiltonian we want to simulate:

$$H_S = \sum_n H_n$$



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Quantum Simulation: Total number of gates vs. depth

Time evolution of the noisy quantum computer:

$$U = e^{i\int_0^t dt(H_{\mathrm{qc}}(t)+H_\gamma)}$$

Simulation with noise:

$$U = e^{iH_S\tau + i\alpha H_\gamma \tau}$$

Scaling factor:

$$\alpha = D\frac{\tau_G}{\tau}$$

Hamiltonian we want to simulate:

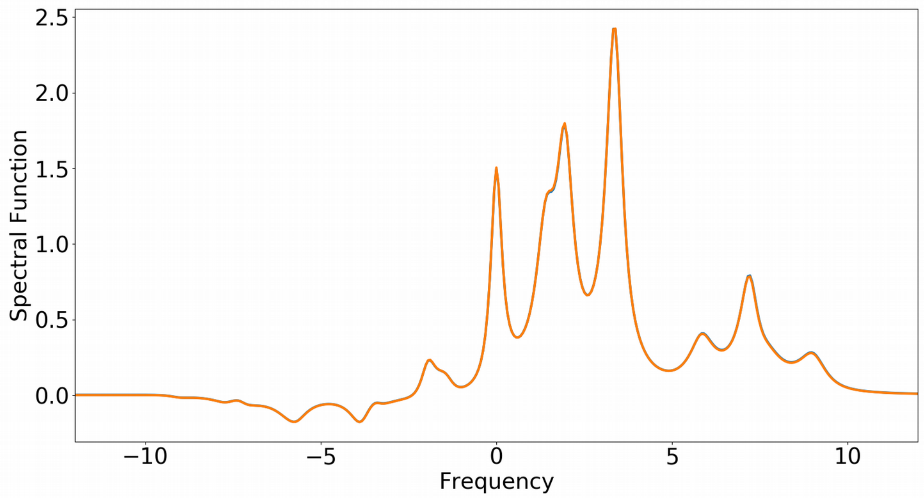
$$H_S = \sum_n H_n = E_{\max}\sum_n h_n \qquad ||h_n|| < 1$$

From this we find a maximal Trotter step size:

$$\tau < \frac{1}{E_{\max}}$$

And we can define the resolution of our simulation:

$$\frac{E_{\min}}{E_{\max}} > \epsilon D$$



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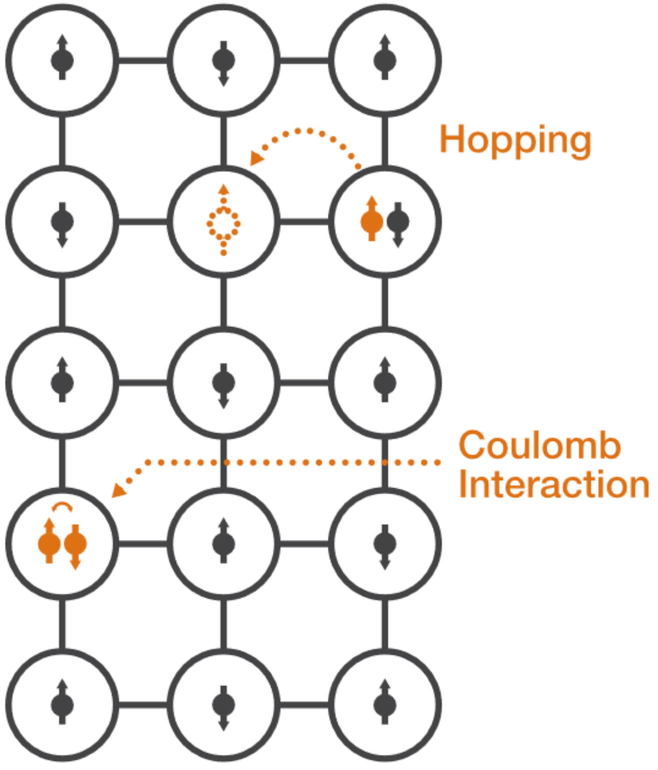
Quantum Simulation: What energies can we resolve?

Example:

Error probability $\epsilon = 1/1000$

Lattice model with 100 Orbitals
and 2D cubic lattice connectivity : $D = 10$

$$\frac{E_{\min}}{E_{\max}} > \frac{1}{100}$$



Hubbard Model

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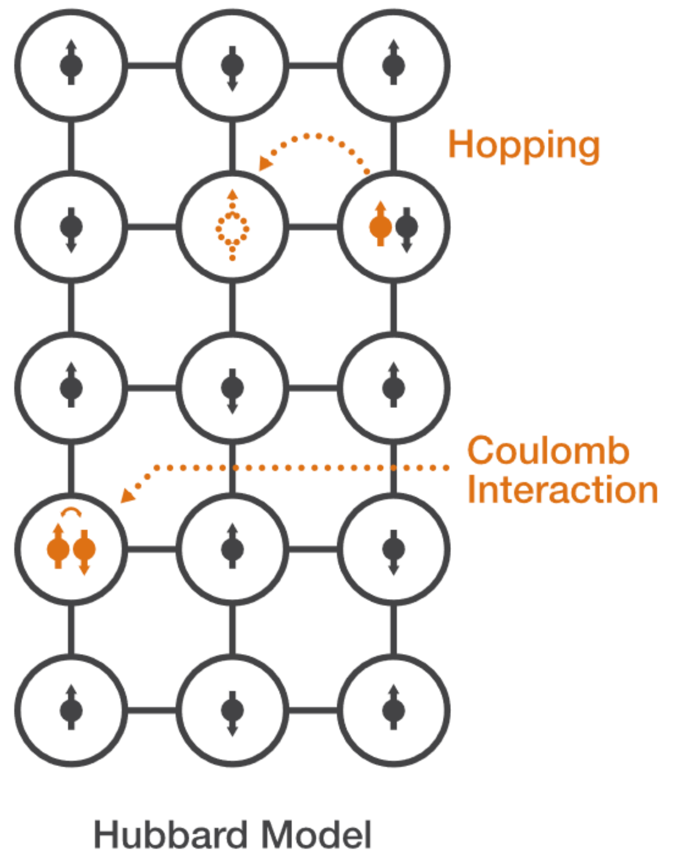
Quantum Simulation: What energies can we resolve?

Example:

Error probability $\epsilon = 1/100$

Lattice model with 50 Orbitals
and all to all connectivity : $D = 50$

$$\frac{E_{\min}}{E_{\max}} > \frac{1}{2}$$



Quantum Simulation: What energies can we resolve?

Example:

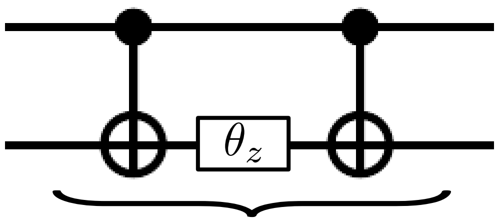
Error probability $\epsilon = 1/100$

Lattice model with 50 Orbitals and all to all connectivity: $D = 50$

$$\frac{E_{\text{min}}}{E_{\text{max}}} > \frac{1}{2}$$

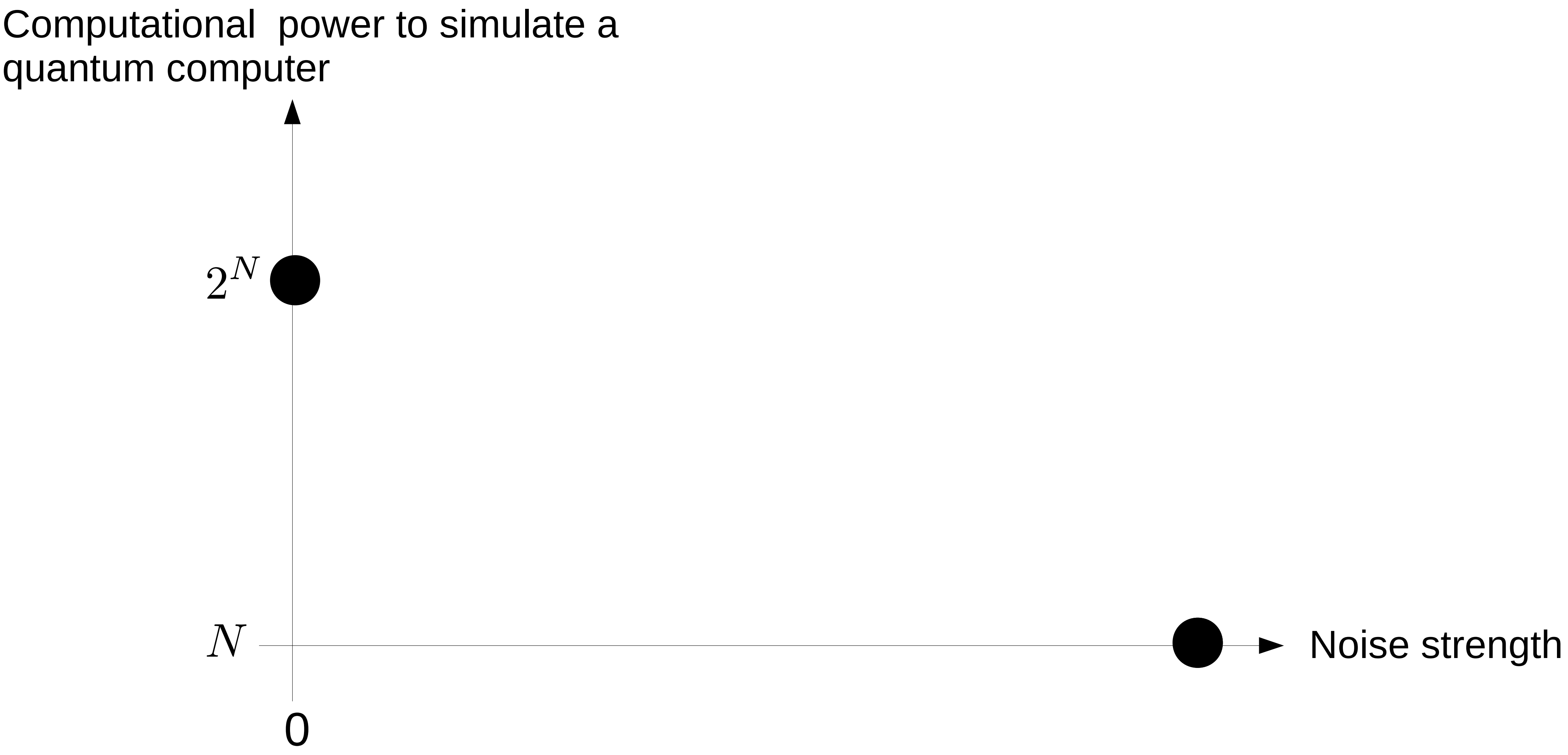
$>$ or $\gg$?

Noise in quantum simulation

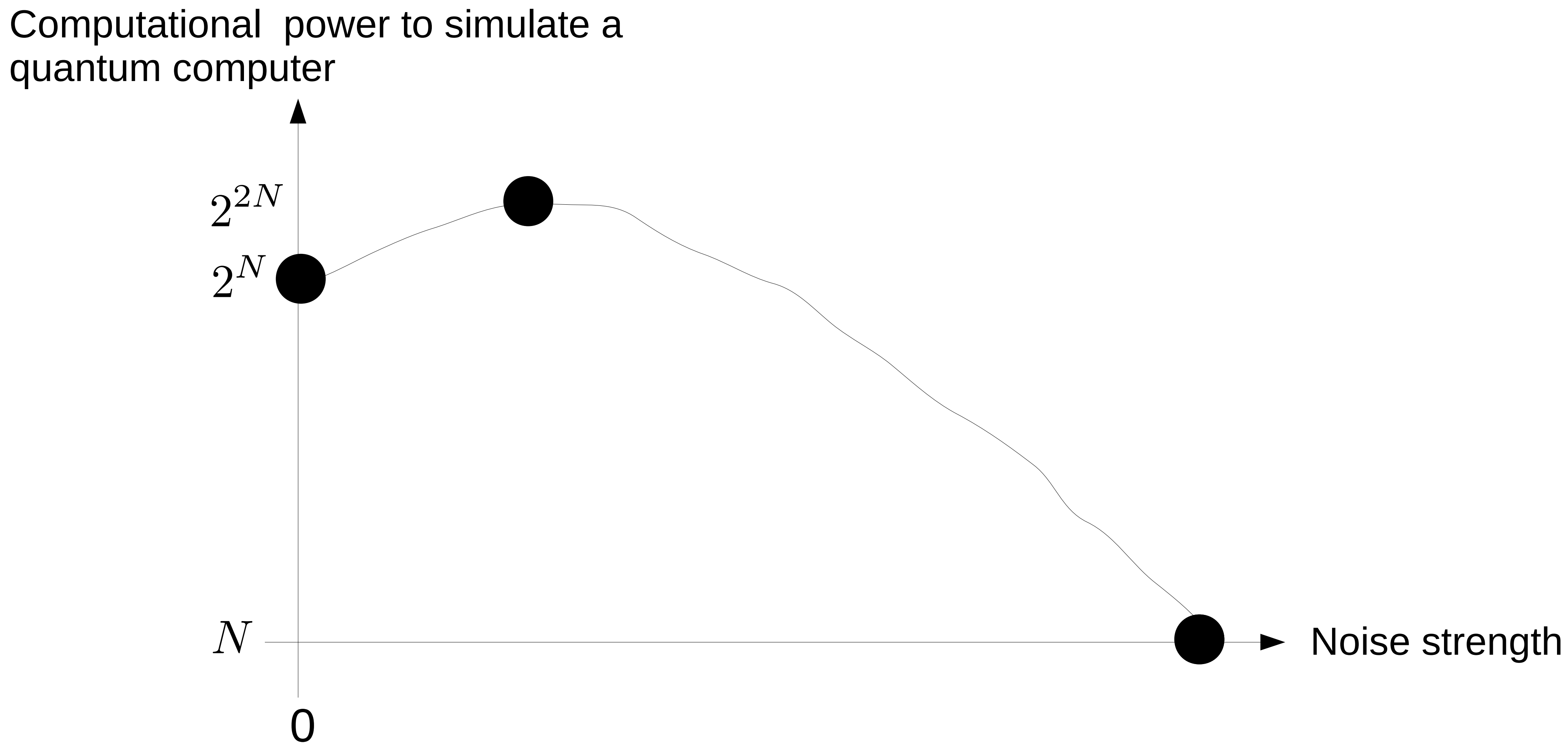


Decoherence during the operation

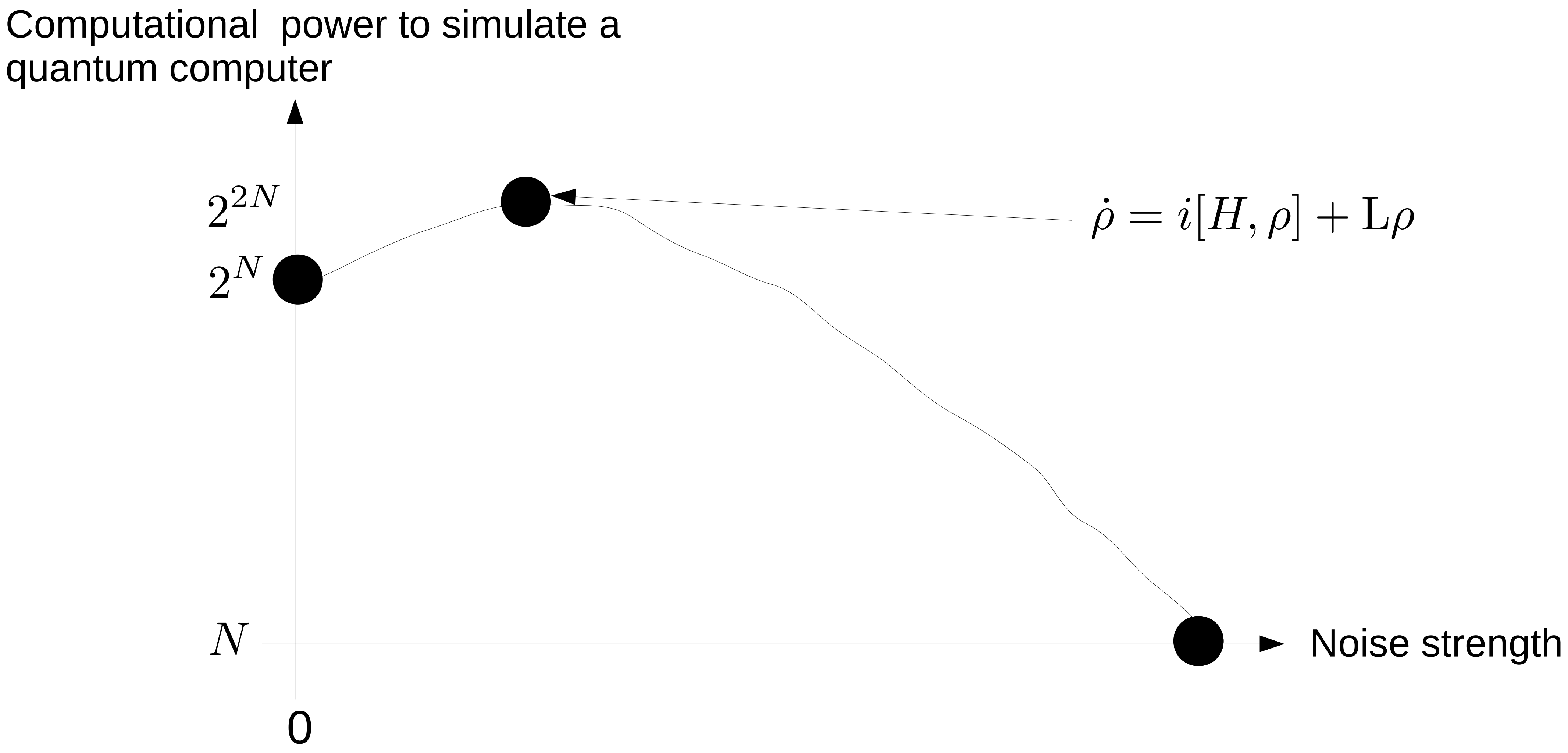
Noise in quantum simulation



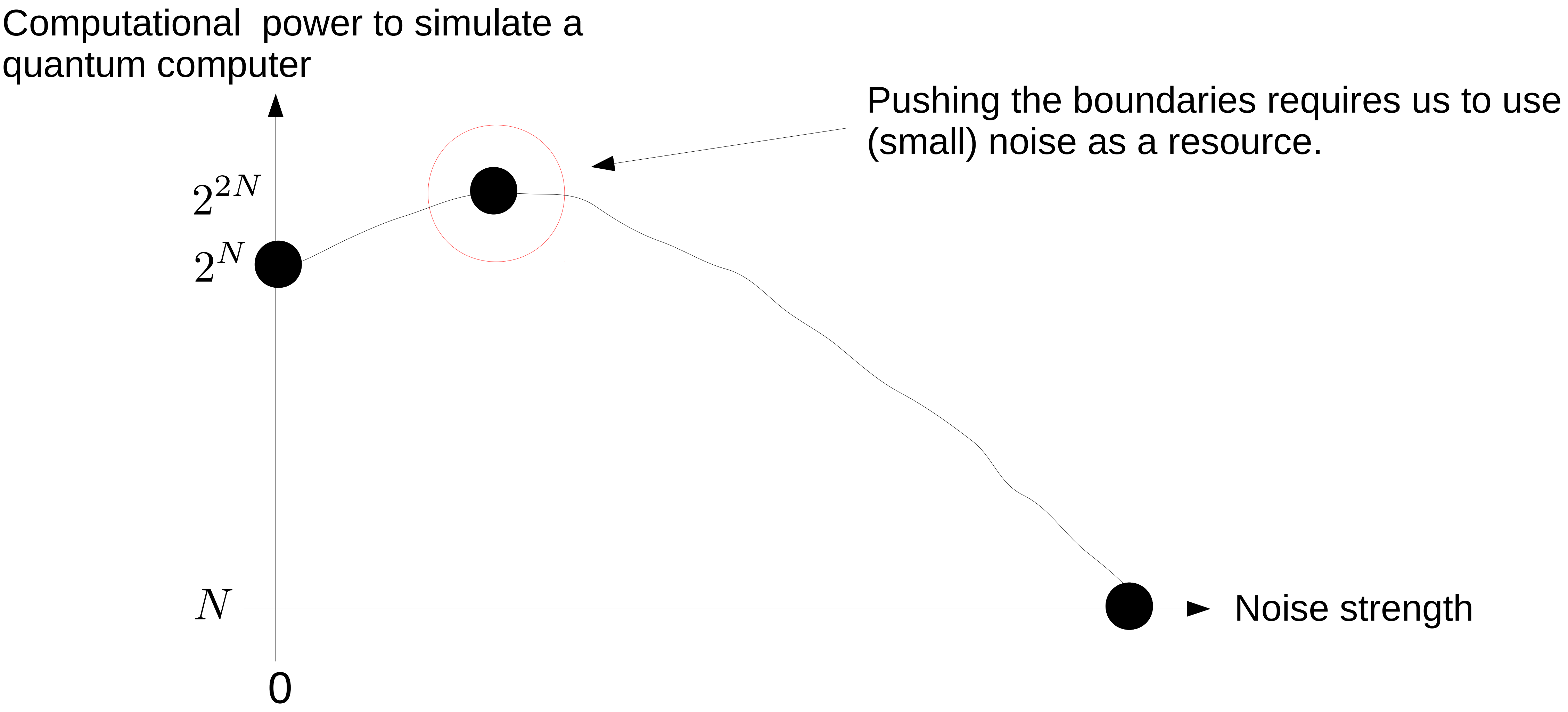
Noise in quantum simulation



Noise in quantum simulation



Noise in quantum simulation



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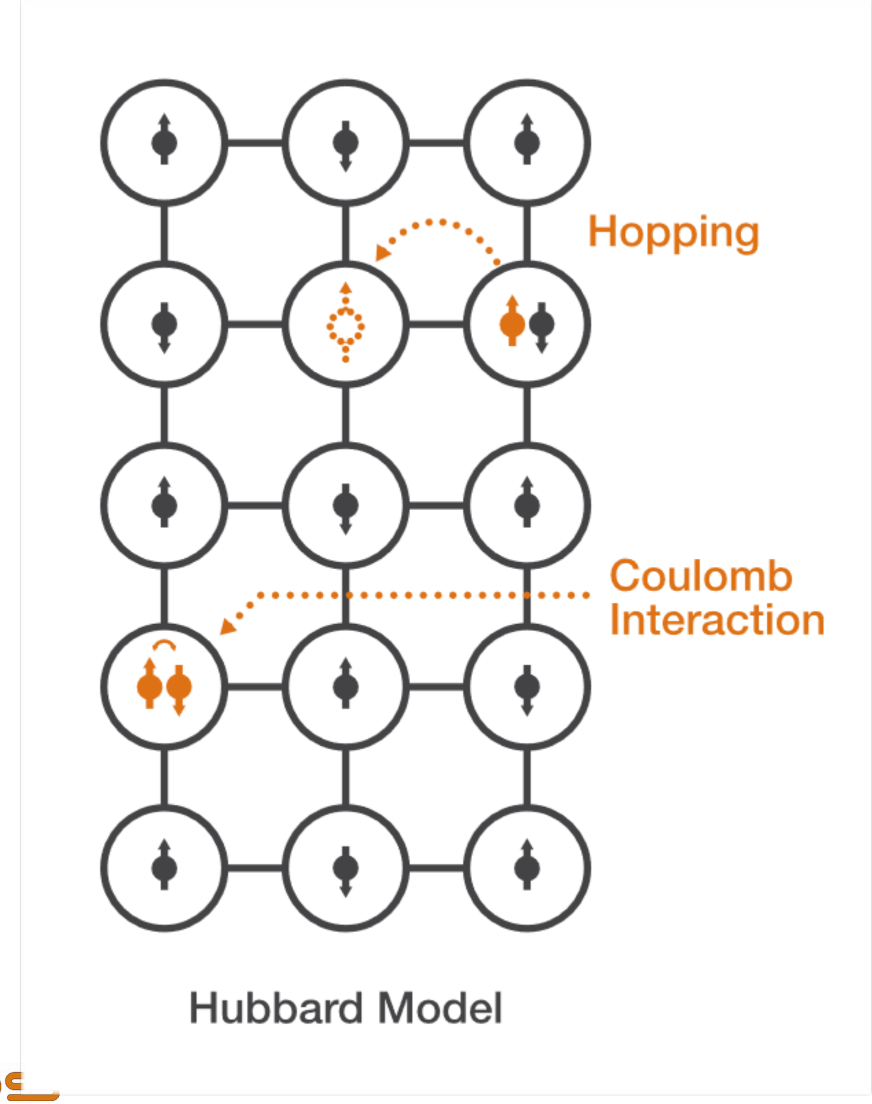
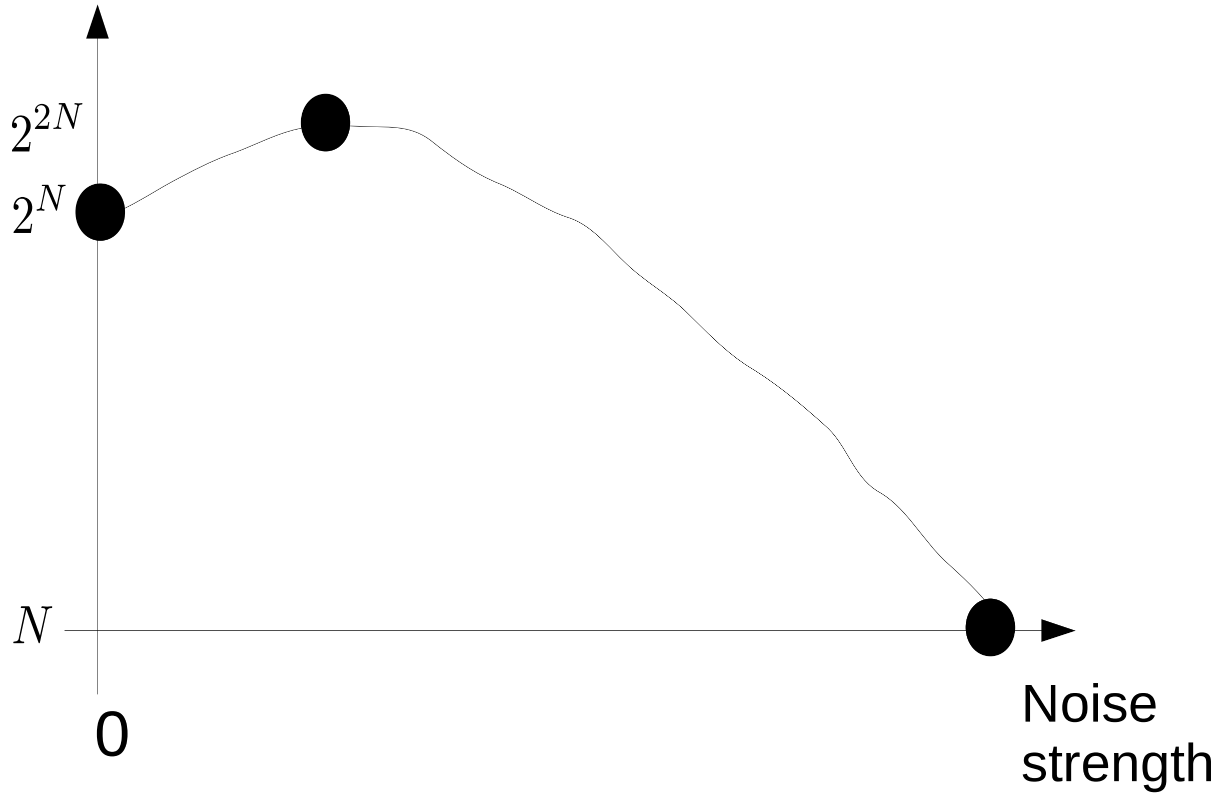
Conclusion



Computational power to
simulate a quantum computer



Thank you!

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