INVESTIGATING SCALING PROPERTIES FOR QUANTUM ANNEALING TO SOLVE THE FERMI-HUBBARD MODEL USING THE KINETIC ENERGY PART AS THE DRIVING HAMILTONIAN

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THE HUBBARD MODEL

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The Hubbard model is an approximate description of interacting electrons in a solid;

$$H = \sum_{i}^{N} \left(\frac{P_i^2}{2m} + V_p(i)\right) + \sum_{i<j}^{N} V_c(i,j)$$

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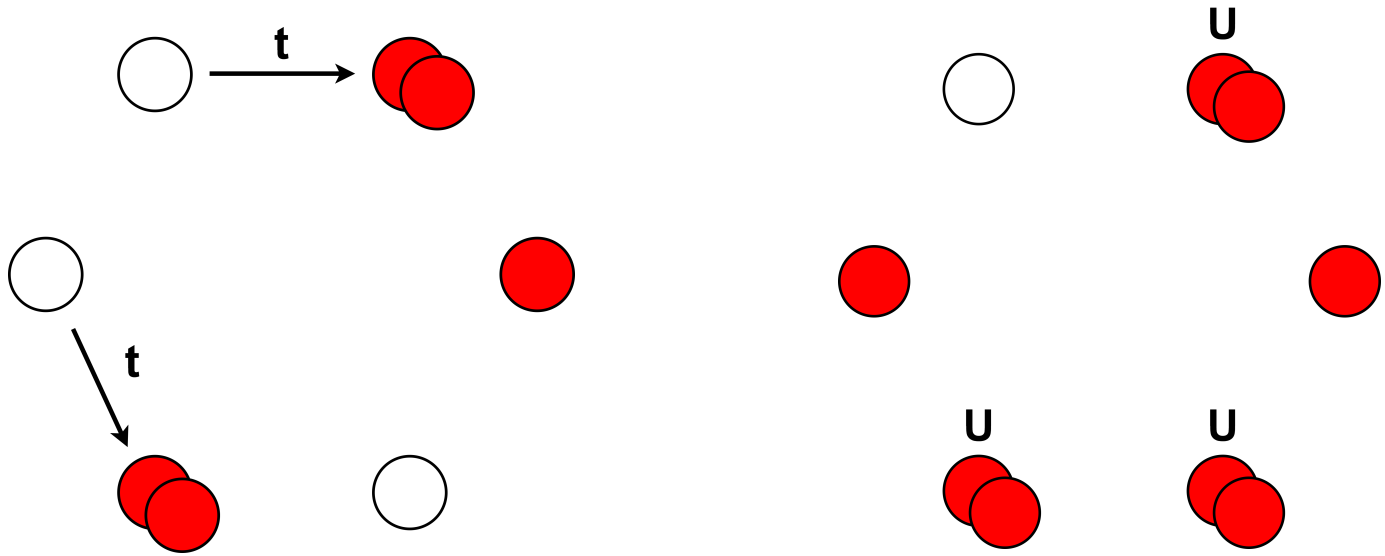
Can adiabatic quantum computing help us circumvent this problem?

THE HUBBARD HAMILTONIAN

L = lattice size
σ = spin index

$$H_H = -t \sum_{\langle i,j \rangle,\sigma}^{L} c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} + u \sum_{i}^{L} n_{i\uparrow} n_{i\downarrow}$$



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$$c_i | \ldots \underbrace{1}_{i} \ldots \rangle = (-1)^x | \ldots \underbrace{0}_{i} \ldots \rangle$$

$$c_i^{\dagger} | \ldots \underbrace{0}_{i} \ldots \rangle = (-1)^x | \ldots \underbrace{1}_{i} \ldots \rangle$$

$$x = \sum_{j}^{i-1} f_j$$

$$n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$$

GROUND-STATE

$L =$ lattice size
$n_{i\sigma} =$ number operator for spin σ

- Exact results only exist for the 1D Hubbard model and numerical calculation of the ground state is exponentially expensive.
- Is there a strategy for quantum annealing that can do better?

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Strategy of adiabatically evolving from a tight binding Hamiltonian to a Hubbard Hamiltonian:

$$H(s) = -t \sum_{\langle i,j\rangle,\sigma}^{L} (c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) + su \sum_{i}^{L} n_{i\uparrow} n_{i\downarrow}$$

$$H(0) = -t \sum_{\langle i,j\rangle,\sigma}^{L} (c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) \xrightarrow{adiabatic} H(1) = H_H$$

ADIABATIC EVOLUTION

$L =$ lattice size
$n_{i\sigma} =$ number operator for spin σ

The adiabatic theorem hints us that:

$$T_A < \int_0^1 \frac{\|\dot{H}\|^2}{\Delta(s)^3} ds \qquad \text{where } \dot{H} = u \sum_i^L n_{i\uparrow} n_{i\downarrow}$$

- scaling of $\Delta(s)$ with system size $\rightarrow$ scaling of T_A required for achieving the ground state
- If $\Delta(s)$ scales $O(L^{-p}) \rightarrow T_A$ scales $O(L^q)$

Since for all s, we have:

$$H(s \neq 0) = H_H(u = su)$$

we look at the behaviour of $min(\Delta(s))$ to infer the scaling behaviour of T_A

Reference $\rightarrow$

HOW?

$L =$ lattice size
$n_{i\sigma} =$ number operator for spin σ

We want to find the ground-state of the half-filled Hubbard Hamiltonian for various values of S_Z;

$$\sum_i^L (n_{i\uparrow} + n_{i\downarrow}) = L \quad \text{and} \quad [\sum_i^L (n_{i\uparrow} - n_{i\downarrow}), H(s)] = 0$$

Lanczos algorithm $\rightarrow$ lower-lying eigenspectrum of $H(s)$

Suzuki-Trotter product formula $\rightarrow$ simulation of time evolution

By doing a diabatic evolution, we can identify the relevant excited states $|\psi_n(s)\rangle$ where;

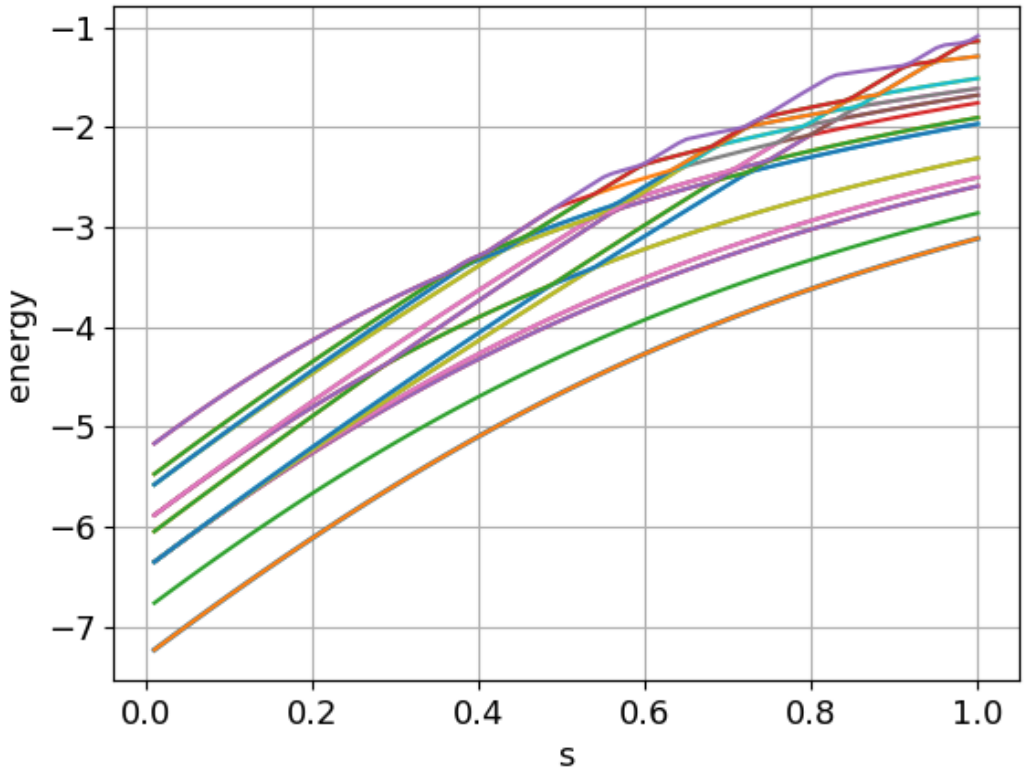
$$\langle \psi_n(s) | U_t(sT_A) | \psi_0(s=0) \rangle \neq 0 \qquad \text{for } n > 0$$

HOW?

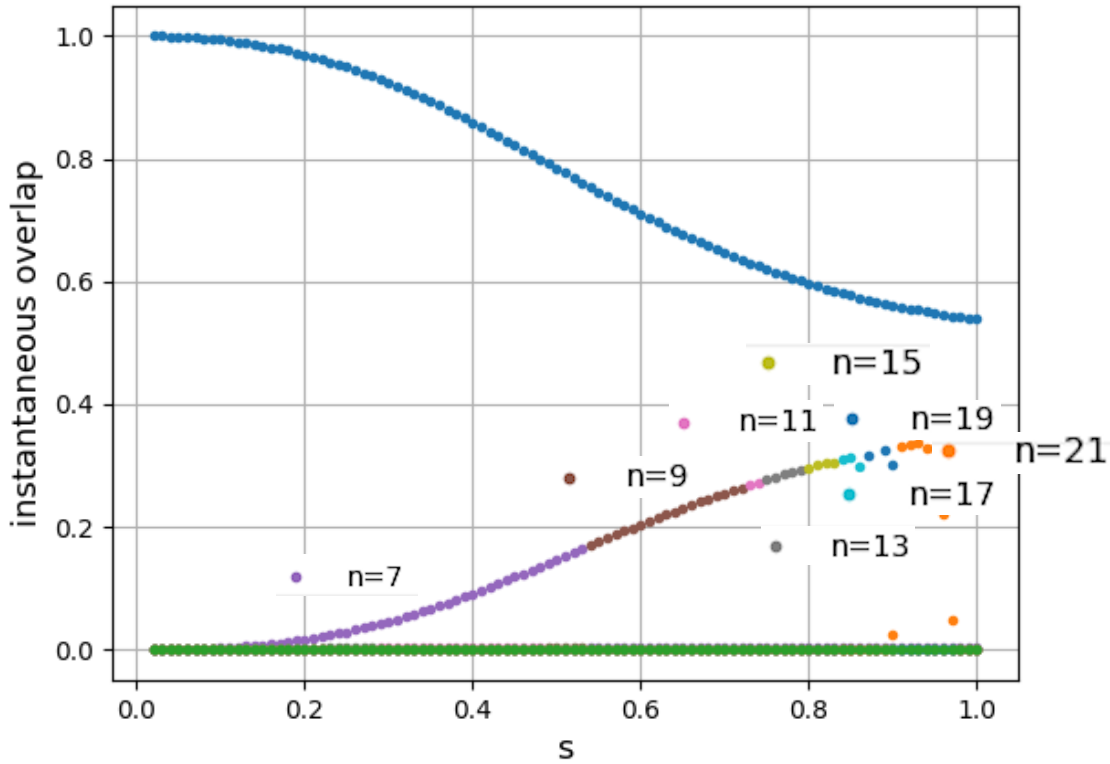
$L =$ lattice size
$n_{i\sigma} =$ number operator for spin σ

$$L = 9, \sum n_{i\downarrow} = 2$$

$E_n(s)$



$|\langle \psi_n(s) | U_t(sT_A) | \psi_0(s=0) \rangle|^2$



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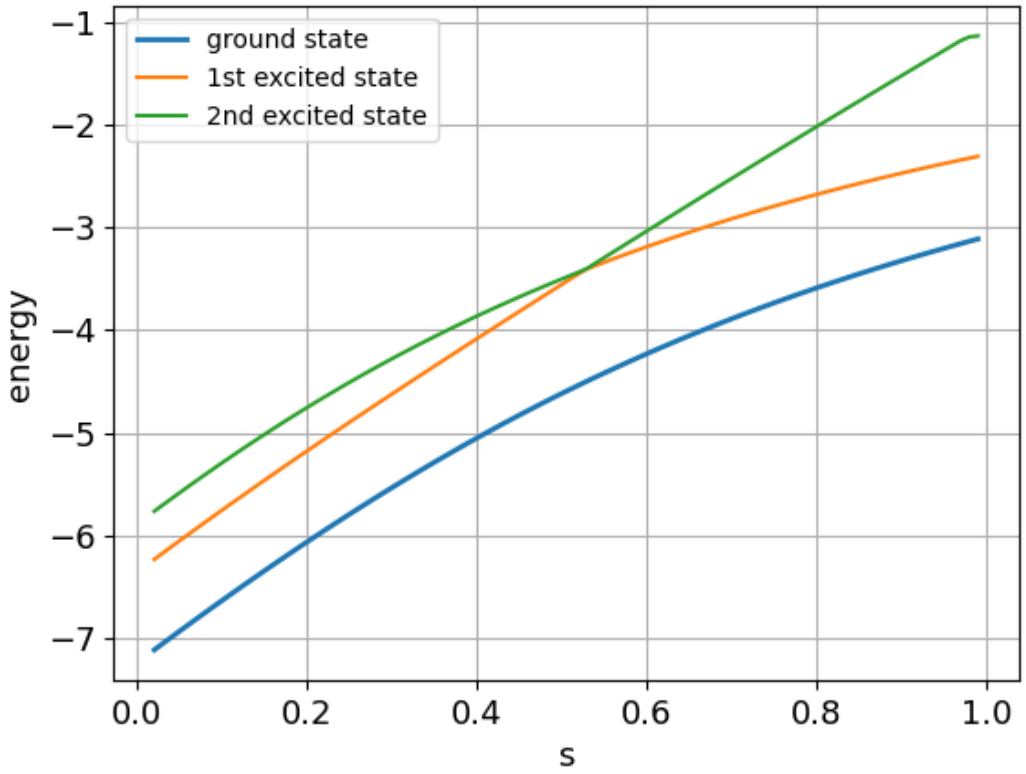
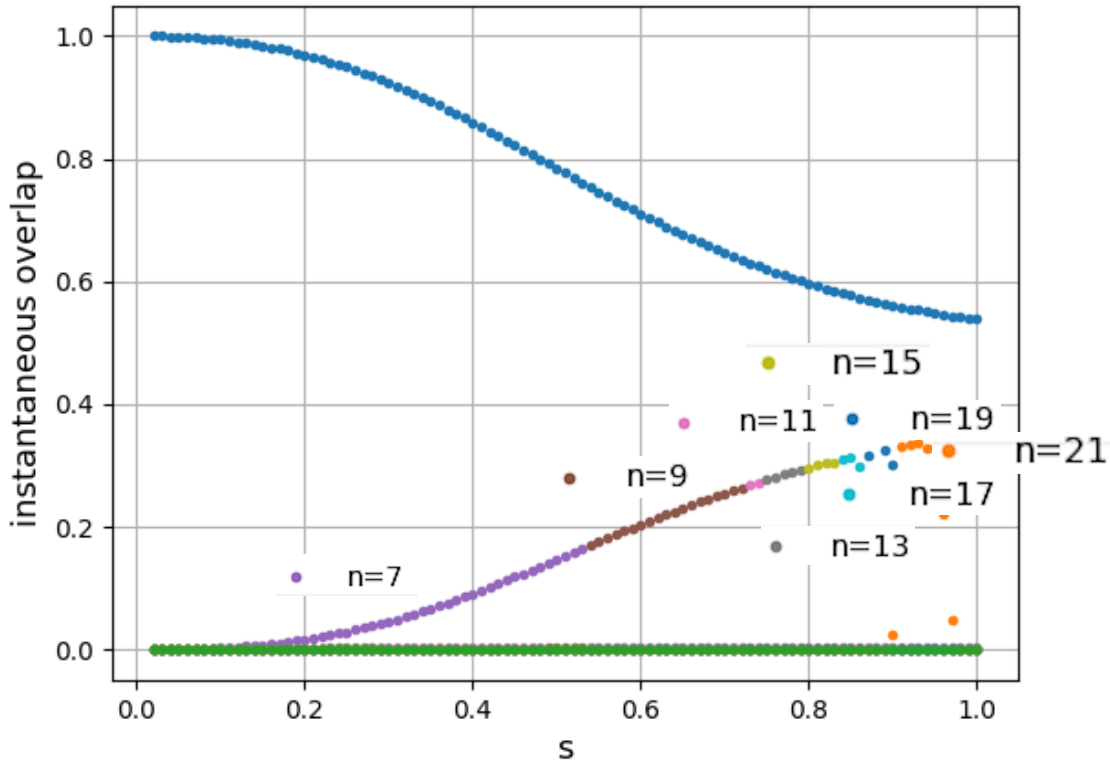


$|\langle \psi_n(s) | U_t(sT_A) | \psi_0(s=0) \rangle|^2$



MINIMUM GAP

$L =$ lattice size
$n_{i\sigma} =$ number operator for spin σ

We are now in a position to determine minimum gap for the problems of our interest;

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We are now in a position to determine minimum gap for the problems of our interest;

1. Calculate $E_n(s)$ for each problem with a given value of L and $\sum_i^L n_{i\downarrow}$

2. Using diabatic excitations, determine which eigenstates are relevant for the given $E_n(s)$

3. Find $min(\Delta(s))$ between $E_0(s)$ and $E_1(s)$

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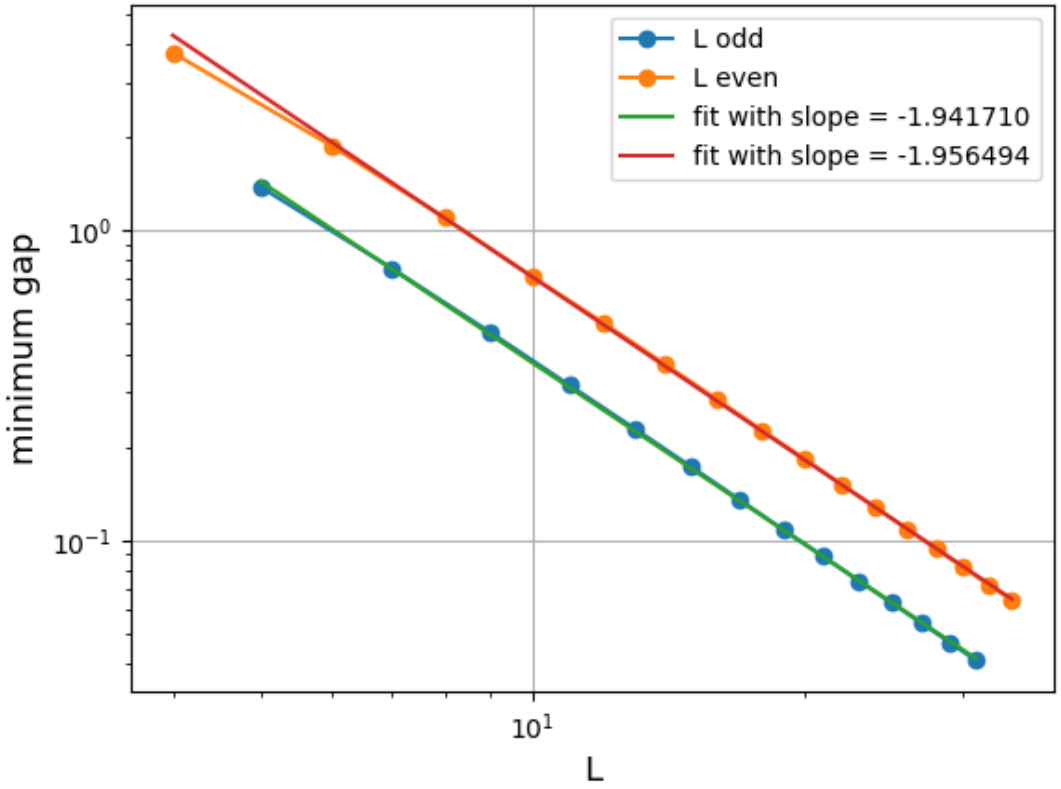
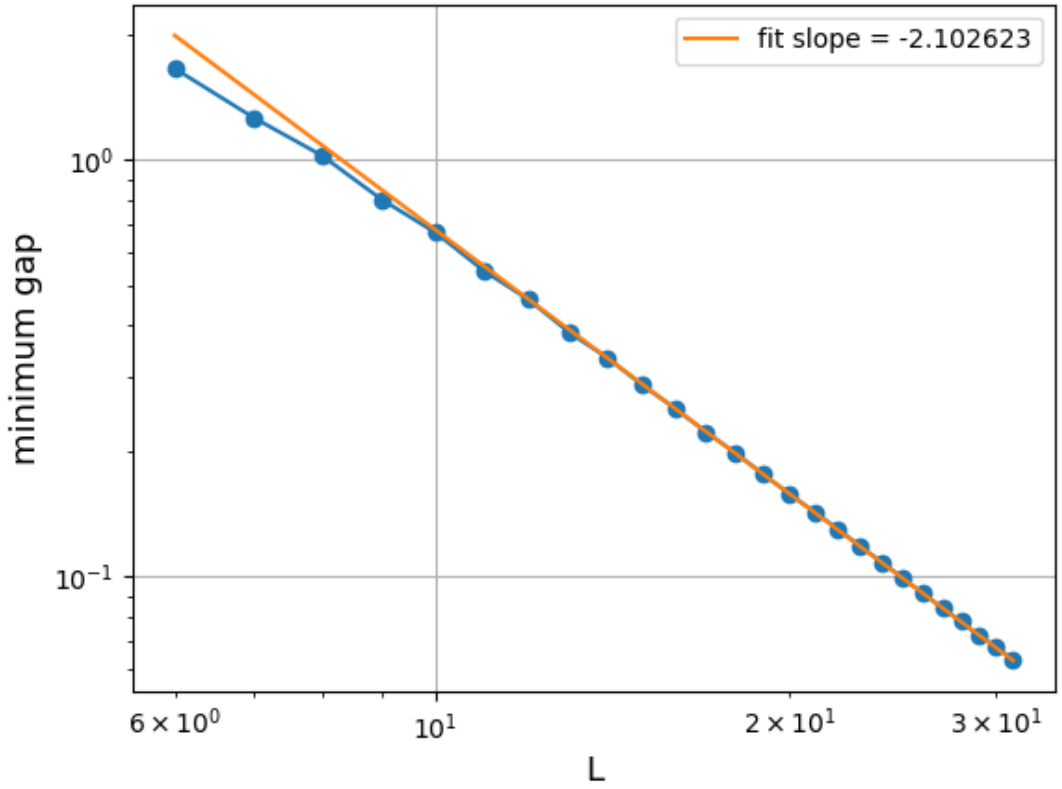




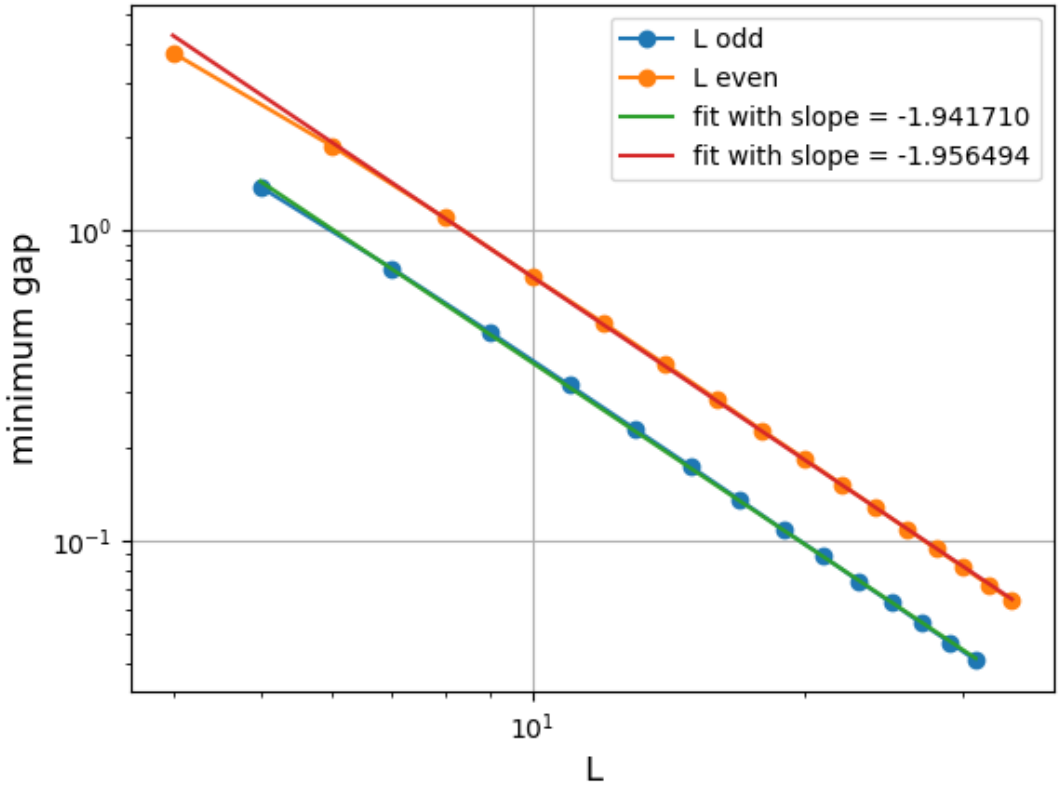
$$\sum n_{i\downarrow} = 1, d \rightarrow O(L^2)$$

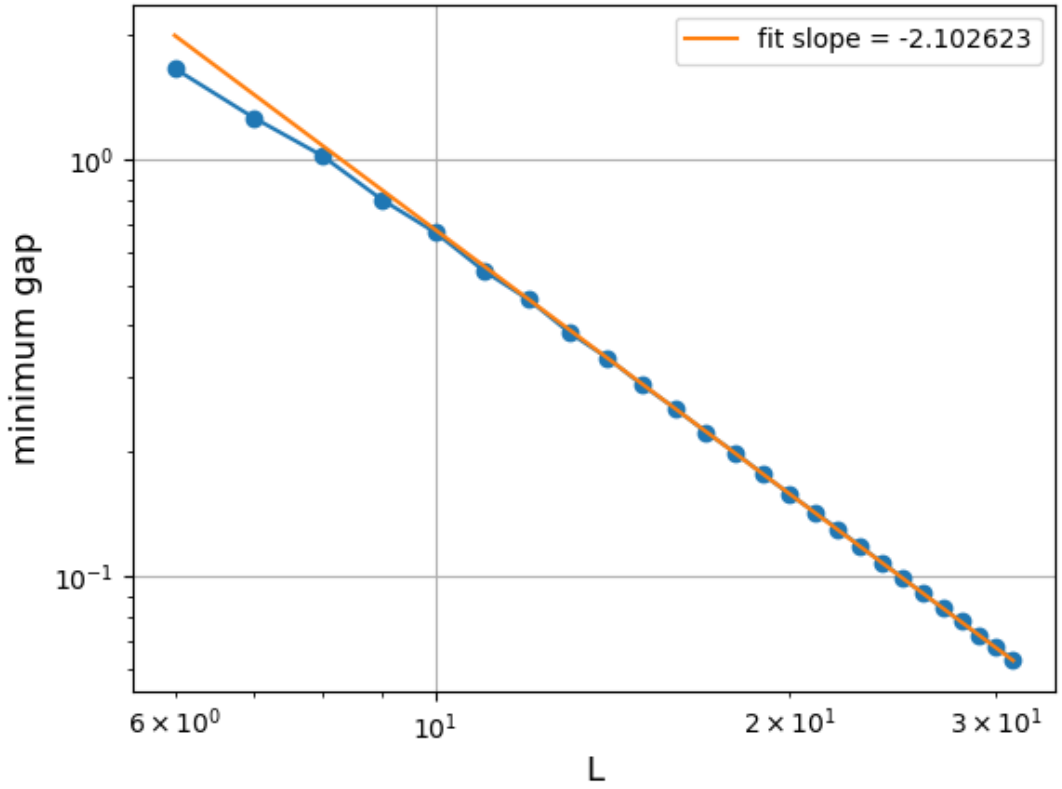
$$\sum n_{i\downarrow} = 2, d \rightarrow O(L^4)$$

MINIMUM GAP

$L =$ lattice size
$n_{i\sigma} =$ number operator for spin σ

$min(\Delta(s))$ vs L for fixed $\sum_{i}^{L} n_{i\downarrow}$ to check for any scaling behaviour





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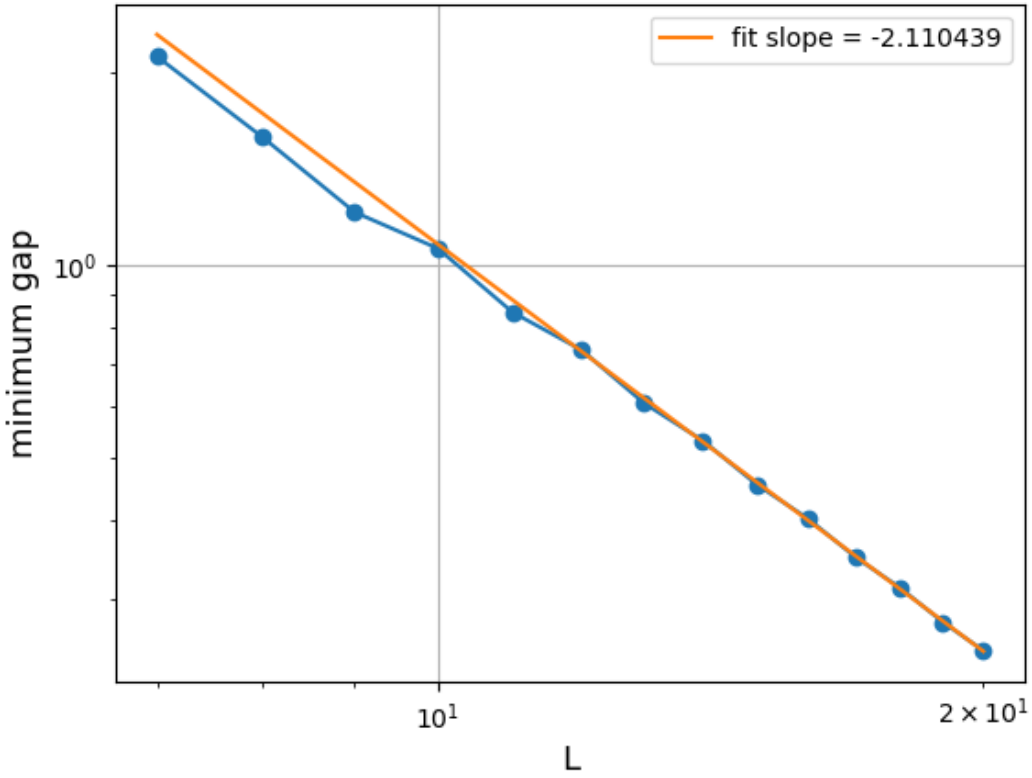

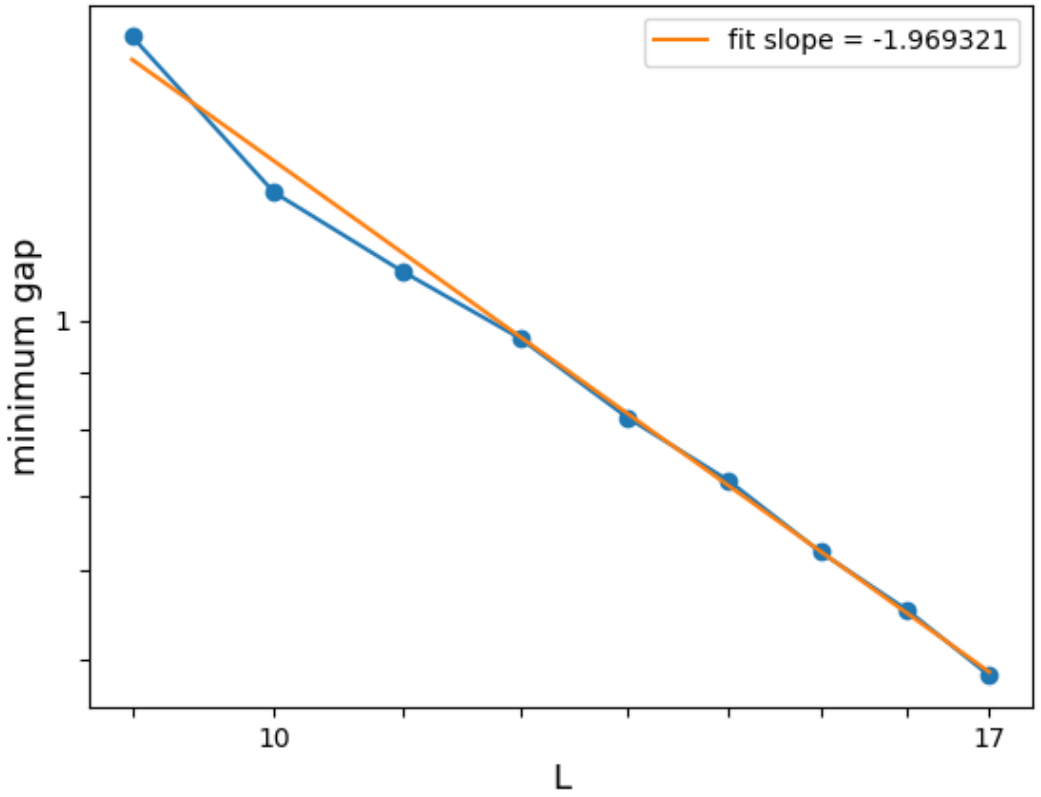

$$\sum n_{i\downarrow} = 3, d \rightarrow O(L^6)$$

$$\sum n_{i\downarrow} = 4, d \rightarrow O(L^8)$$

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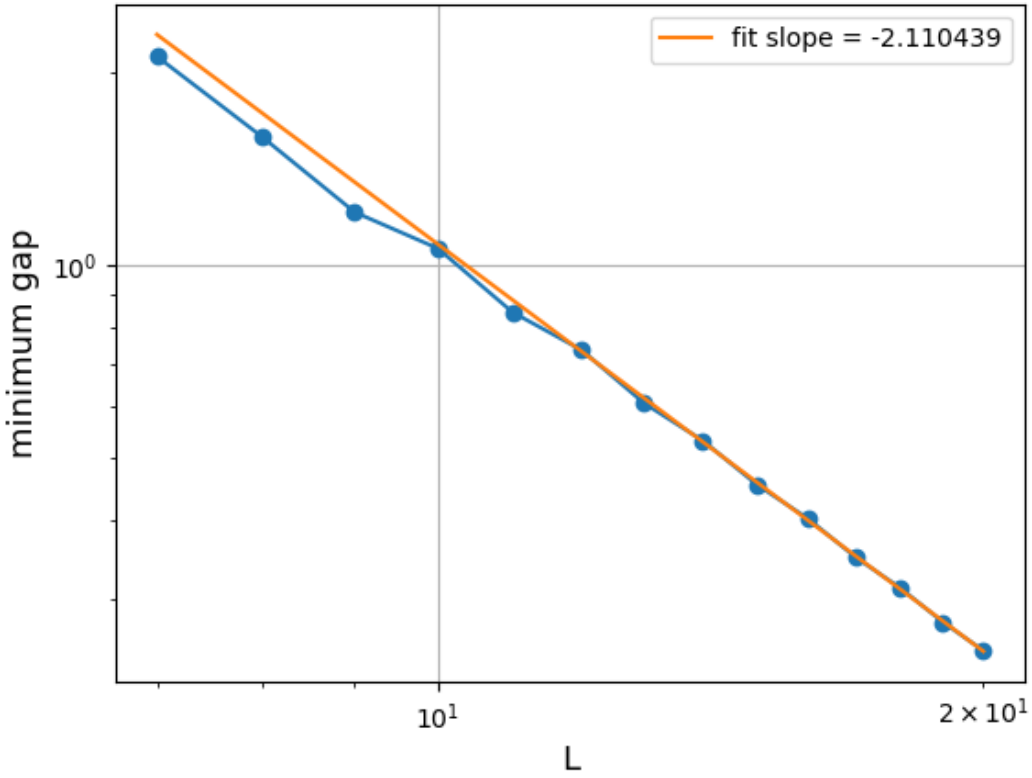
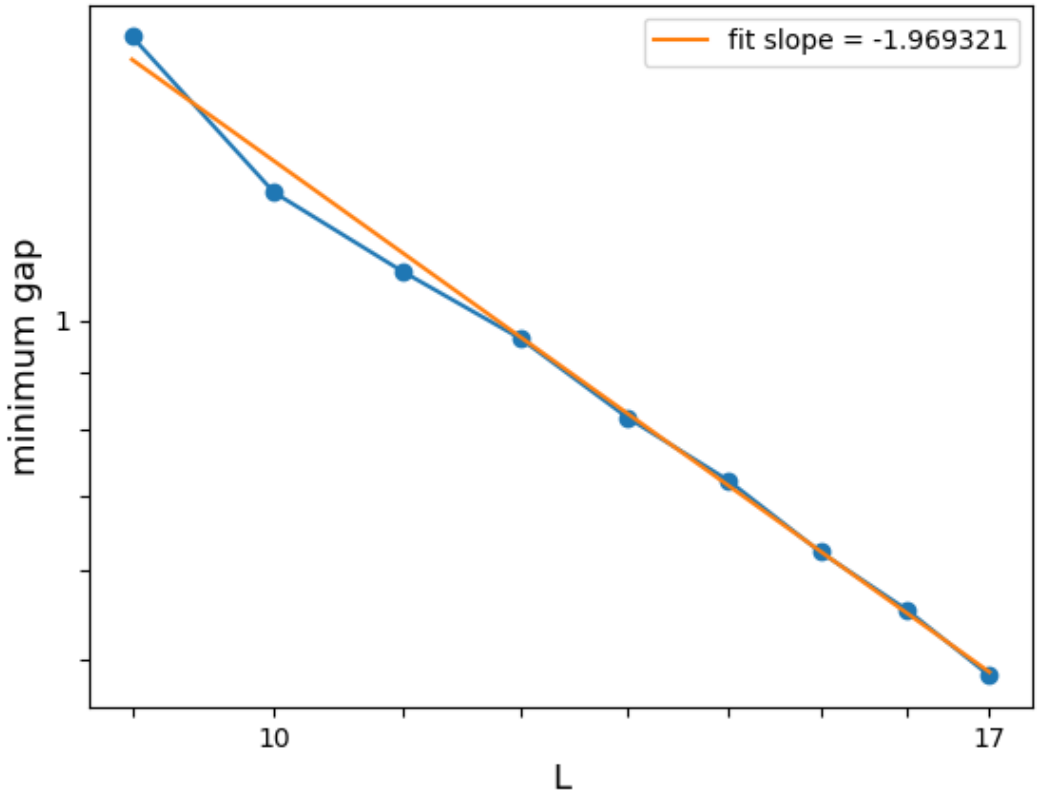
$min(\Delta(s))$ vs L for fixed $\sum_{i}^{L} n_{i\downarrow}$ to check for any scaling behaviour





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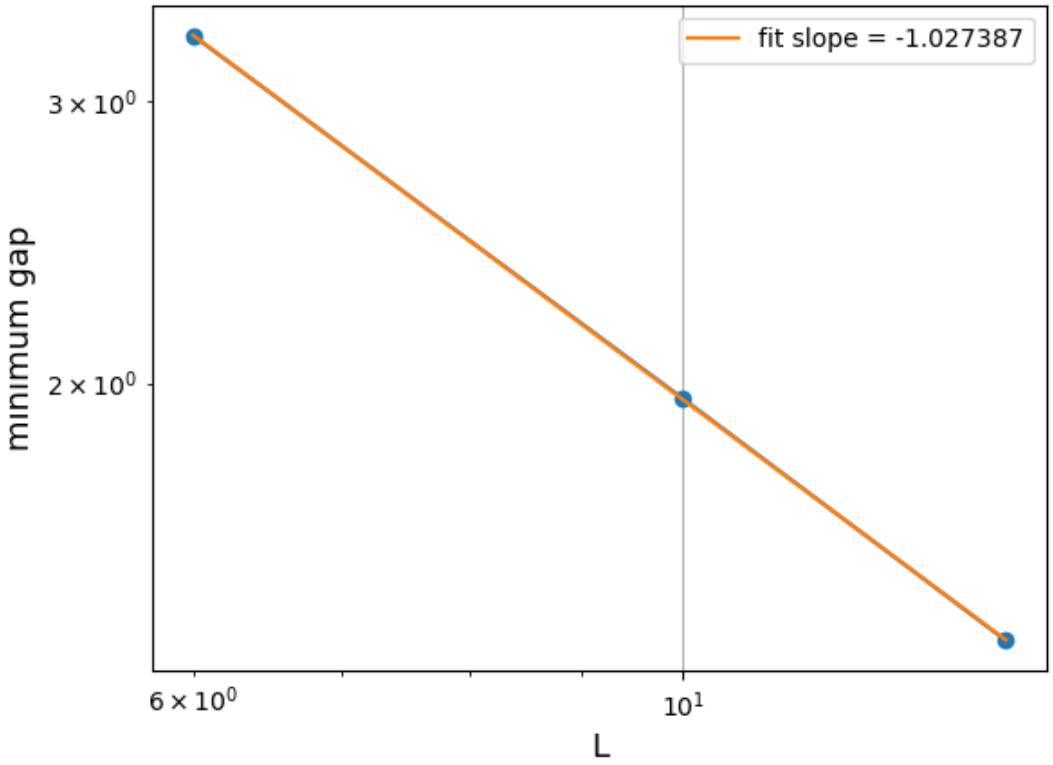

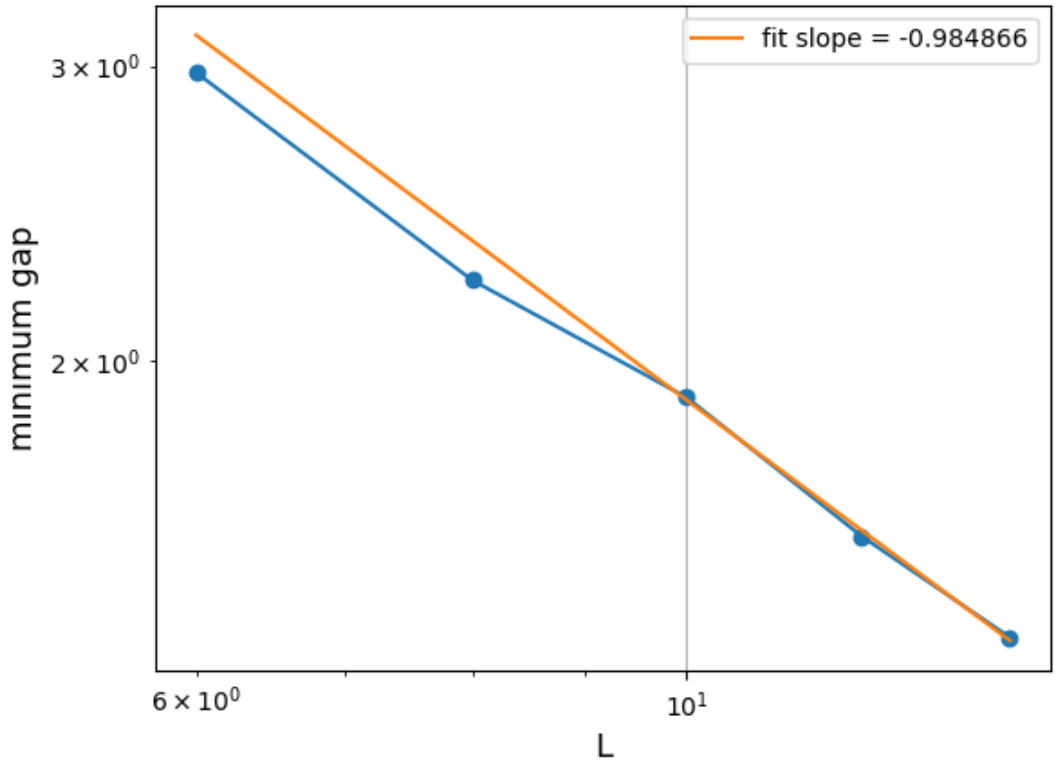

$$\sum n_{i\downarrow} = L/2, d \rightarrow O(4^n)$$

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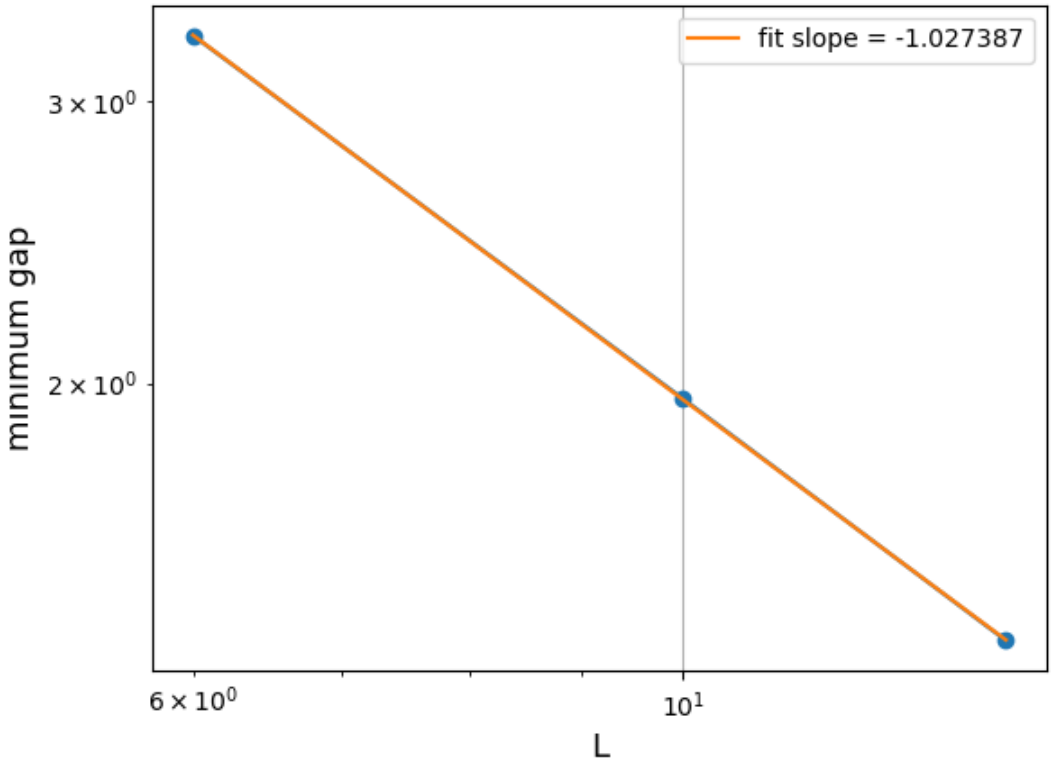

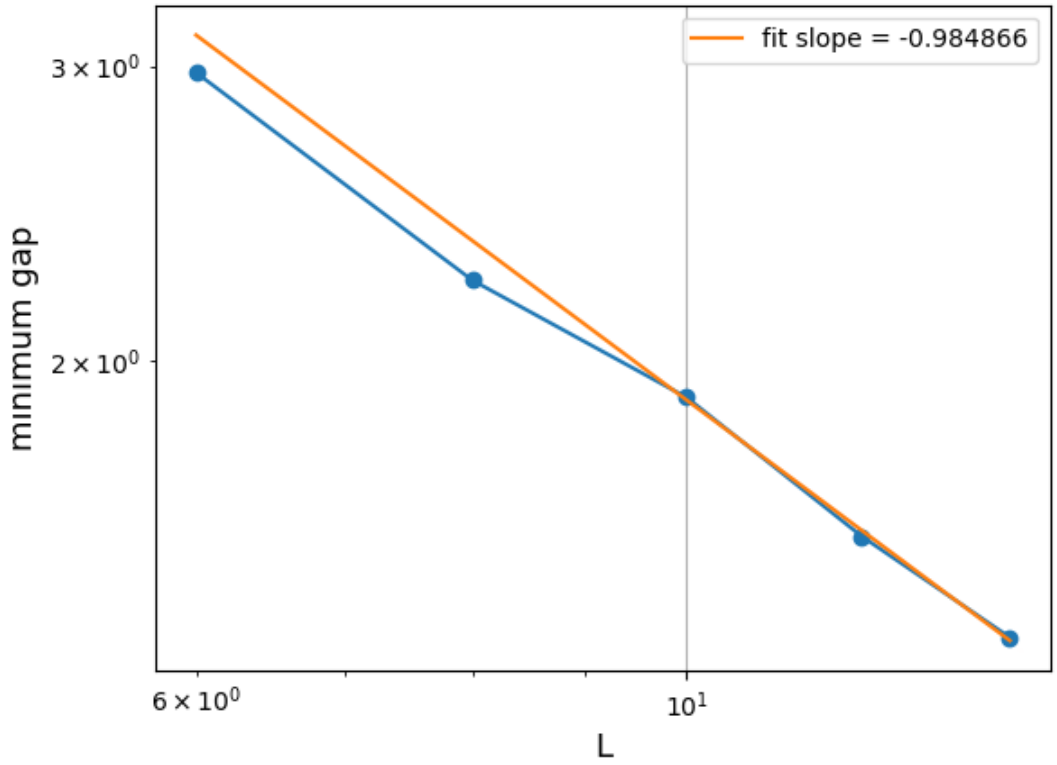

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LADDER GEOMETRY

$L =$ lattice size
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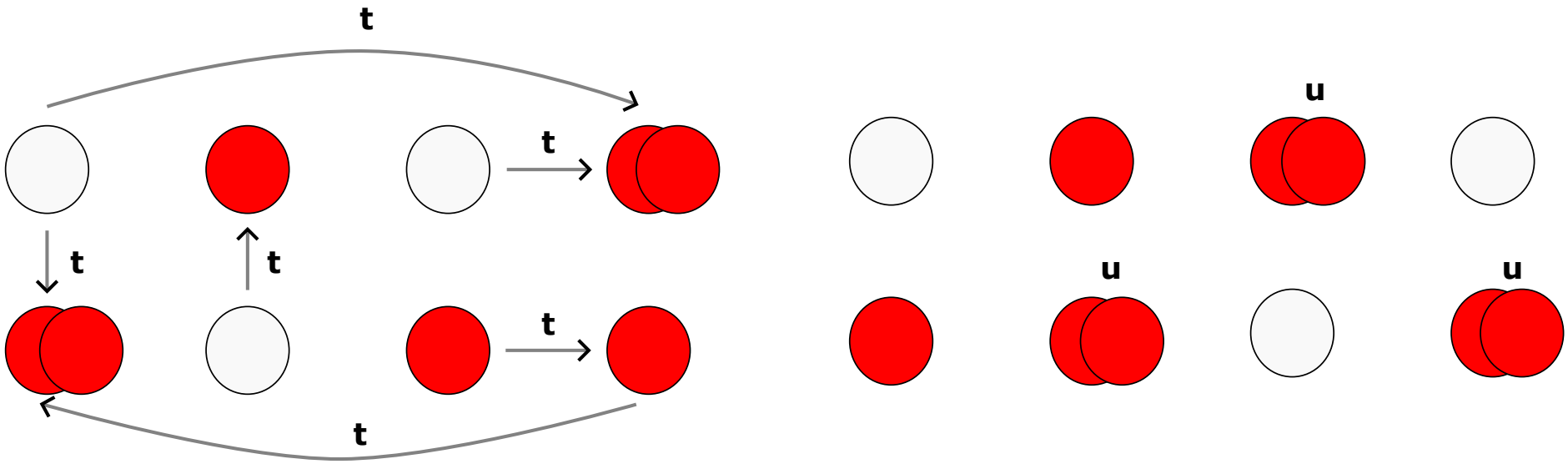
Since the Hubbard model on a ladder is not exactly solved, we also tried to see if there is a similar behaviour for it

$$H_H = -t \sum_{\langle i,j \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} + u \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



MINIMUM GAP(LADDER)

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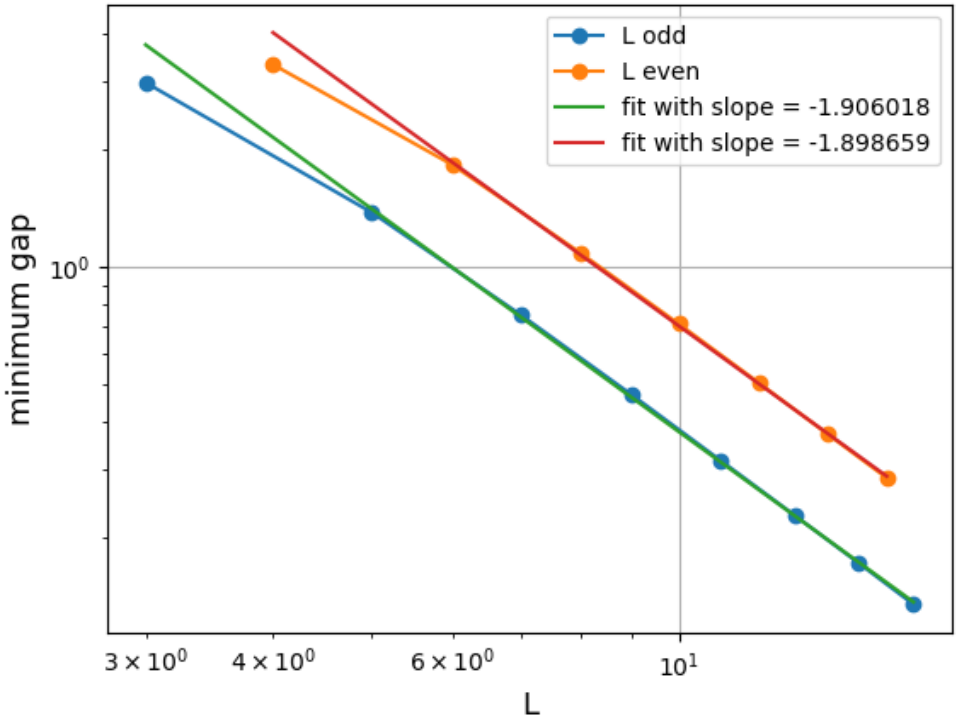

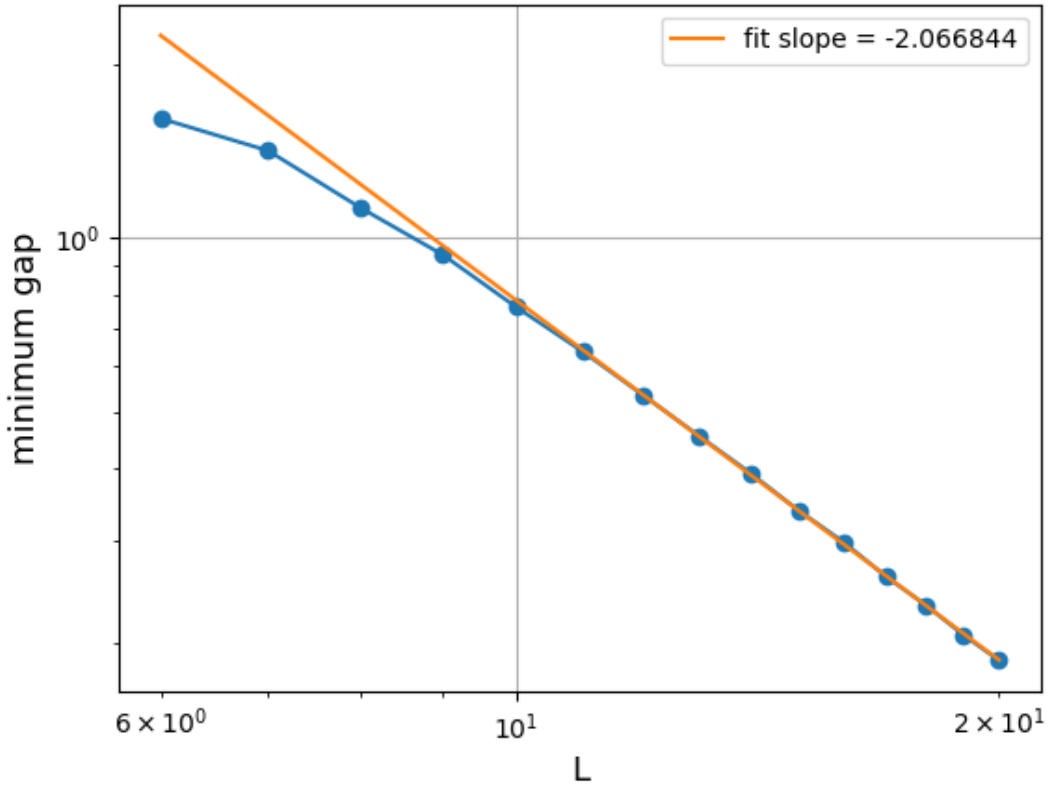

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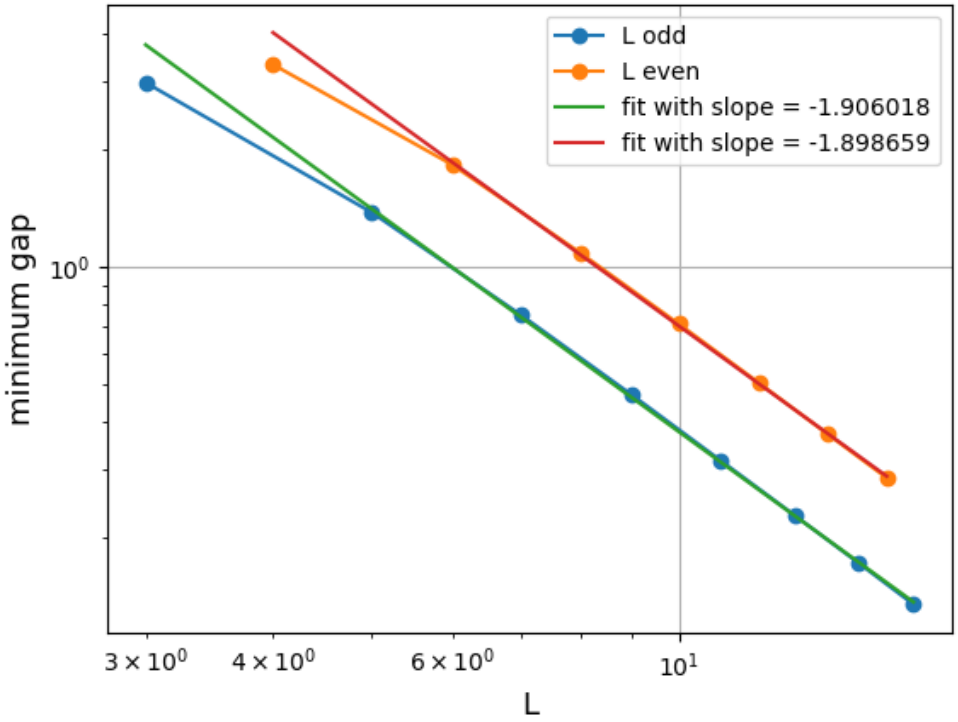

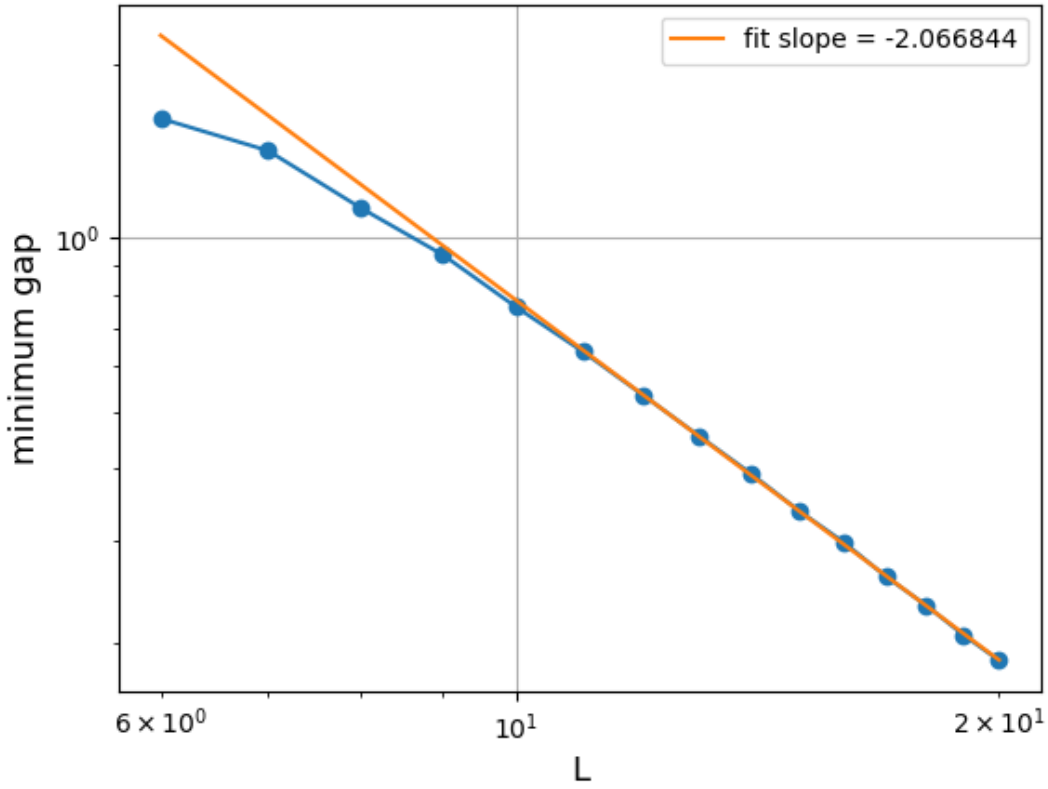

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WHAT CAN WE SAY?

$L =$ lattice size
$n_{i\sigma} =$ number operator for spin σ

$$min(\Delta(s)) \sim \frac{1}{L^2} \text{ for fixed } \sum_{i}^{L} n_{i\downarrow}?$$

- If this trend holds for large values of $\sum n_{i\downarrow}$, it might mean that the ground-state of the Hubbard model can be achievable in polynomial time
- This encourages us to look further into the utility of adiabatic quantum computation for solving the Hubbard model
- The next step would be to do gate based simulations of quantum annealing to explore further

JUQCS

Jülich Quantum Computer Simulator

- High-performance program for simulating all kinds of gate based circuits
- Can simulate circuits for upto 42 qubits

Idea?

1. Study the quantum annealing behaviour for a system as large as possible
2. Look at the feasibility from a gate-based perspective

Initial steps?

1. Determine circuit for preparing initial state
2. Prepare circuit for Suzuki-Trotter steps of adiabatic time evolution
3. Prepare measurement procedure
4. Bring it all together

INITIAL STATE PREPARATION

$N =$ no. particles
$m =$ number of givens rotations

$$\underbrace{c_{i_1}^\dagger \dots c_{i_N}^\dagger |0\rangle}_{\text{easy-to-prepare}} \rightarrow \underbrace{c_{k_1}^\dagger \dots c_{k_N}^\dagger |0\rangle}_{\text{initial ground-state}}$$

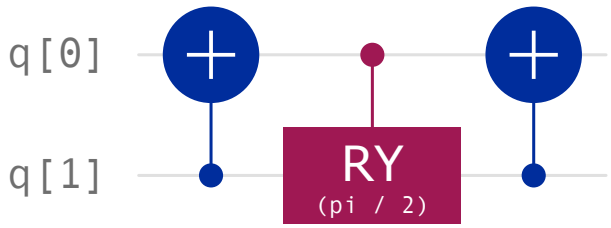
$$\begin{pmatrix} c_{i_1}^\dagger \\ \cdot \\ c_{i_N}^\dagger \end{pmatrix} = Q \begin{pmatrix} c_{k_1}^\dagger \\ \cdot \\ c_{k_N}^\dagger \end{pmatrix}$$

It turns out; $Q = G_1 G_2 \dots G_m$ where $G(\theta) = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}$

Givens rotations on neighbouring rows!

If two neighbouring spin orbitals are considered;

$$G(\frac{\pi}{2}) \begin{pmatrix} c_j^\dagger \\ c_{j+1}^\dagger \end{pmatrix} \rightarrow$$



Reference →

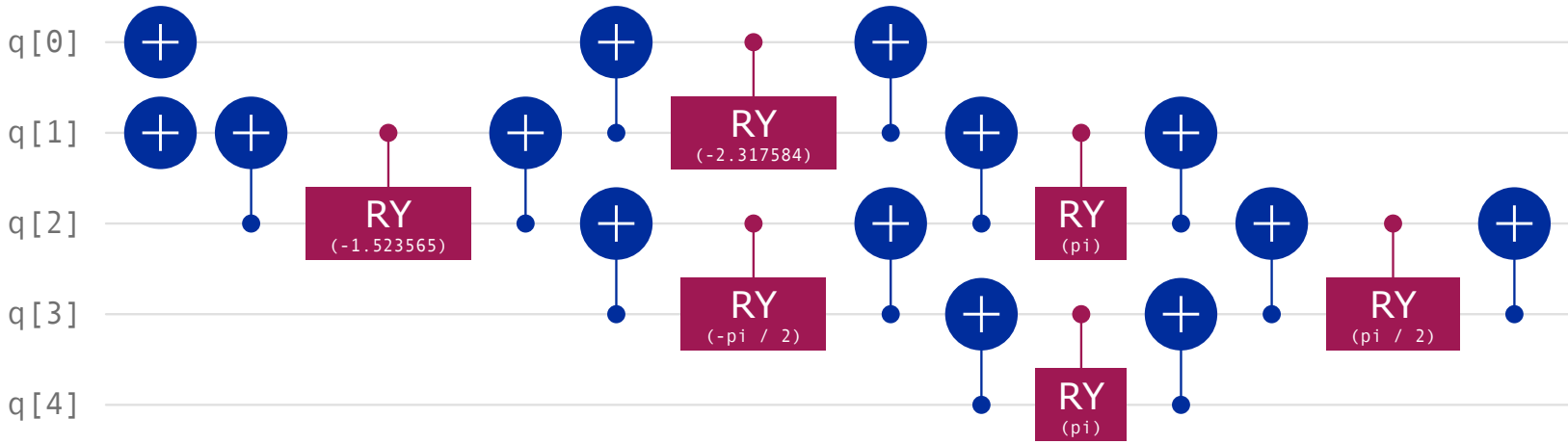
INITIAL STATE PREPARATION

Given Q, the sequence of givens rotations can be calculated in an efficient way as shown in the reference;

$$m = (L - \sum_i^L n_{i\downarrow}) \sum_i^L n_{i\downarrow} + (L - \sum_i^L n_{i\uparrow}) \sum_i^L n_{i\uparrow}$$

$$\text{Depth} = L - 1$$

Q = transformation matrix
L = lattice size
m = number of givens rotations



Circuit for preparing the initial ground state for $L = 5, \sum_i^L n_{i\downarrow} = 2$

TIME-EVOLUTION ON A QUANTUM COMPUTER

$$e^{-i\tau u n_{i\downarrow} n_{i\uparrow}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{-i\tau u} \end{pmatrix}$$

$$e^{-i\tau t(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma})} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(i\tau t) & (-1)^x \sin(i\tau t) & 0 \\ 0 & (-1)^x \sin(i\tau t) & \cos(i\tau t) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$x = \sum_{s=i+1}^{j-1} f_s$$

Suzuki-Trotter steps → building blocks of time evolution

Various ways of constructing appropriate circuits

Depth increases due to parity in hopping term

Depth of Suzuki-Trotter step → $O(L)$
Can be reduced

SUMMARY

$L =$ lattice size
$T_A =$ annealing time

- Circuits for state preparation and time-evolution steps have depth $O(L)$
- If $T_A \sim O(L^2)$ can be established for the Hubbard model, then it is an indication of quantum adiabatic computing to be a natural platform for solving such models
- This bolsters our hope towards the promise of quantum computers and encourages us to try harder to establish its advantages

THANK YOU VERY MUCH!