FINDING THE GROUND STATE OF THE 1D HUBBARD MODEL USING QUANTUM ANNEALING

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$L =$ lattice size

The Hubbard model

The 1-dimensional Hubbard Hamiltonian with open boundaries and nearest neighbour hopping:

$$H_H = -t_H \sum_{\substack{i=1 \\ \sigma=\uparrow,\downarrow}}^{L-1} (c^\dagger_{i\sigma} c_{i+1\sigma} + c^\dagger_{i+1\sigma} c_{i\sigma}) + U \sum_{i}^{L} n_{i\uparrow} n_{i\downarrow}$$

- Foundational model to capture some qualitative behaviour of correlated fermions on a lattice.
- Ground-state properties of the Hamiltonian describe the behaviour.

How hard is it to find this ground-state?

$L =$ lattice size

Classical algorithms

Exact diagonalization

- Exact calculation of the eigenvalues and eigenvectors of H_H.
- Hilbert space dimension (D) for N fermions and $N_\downarrow$ spin-$\downarrow$ fermions

$$D = \binom{N}{N_\downarrow}^2 .$$

- Memory: $O(D^2)$, Number of operations: $O(D^3)$

Lanczos algorithm

- Finding the low lying eigenstates and eigenvalues by repeated application of $H_H|\psi\rangle$.
- Memory: $O(nD)$, Number of operations: $O(nLD)$, where n is the number of Lanczos iterations.

$L =$ lattice size

Classical algorithms

Bethe-ansatz equations

Non-linear algebraic equations for quantum numbers $\{k_1, k_2 \ldots k_N\}$ and $\{\lambda_1, \lambda_2 \ldots \lambda_{N_\downarrow}\}$.

$$2k_j(L+1) = 2\pi I_j + \sum_{b=\pm 1} \sum_{r=1}^{N_\downarrow} \phi(2\sin k_j + 2b\lambda_r)$$

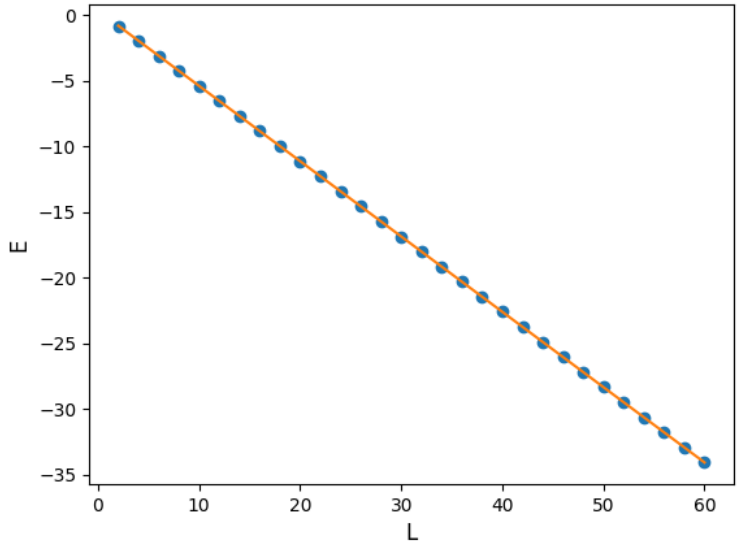
where $\phi(x) = -2\arctan(2x/U)$

$$\sum_{b=\pm 1} \sum_{l=1}^{N} \phi(2b\sin k_l + 2\lambda_r) = -2\pi J_r + \sum_{b=\pm 1} \sum_{s\neq 1}^{N_\downarrow} \phi(\lambda_r + b\lambda_s)$$

$I_j = j, J_r = r$ for ground-state

$$E = -2\sum_{j=1}^{N} \cos k_j$$

$\frac{3L}{2}$ equations for a half-filled lattice $(2N_\downarrow = N = L)$



- Need to be solved numerically for finite L
- Root finding → **polynomial time in** L

$L =$ lattice size

Quantum annealing

Strategy of adiabatically evolving from the kinetic energy part to the full Hubbard Hamiltonian:

$$H(s) = -t_H \sum_{\substack{i=1 \\ \sigma=\uparrow,\downarrow}}^{L-1} (c_{i\sigma}^{\dagger} c_{i+1\sigma} + c_{i+1\sigma}^{\dagger} c_{i\sigma}) + sU \sum_{i}^{L} n_{i\uparrow} n_{i\downarrow}$$

$$H(0) = -t_H \sum_{\substack{i=1 \\ \sigma=\uparrow,\downarrow}}^{L-1} (c_{i\sigma}^{\dagger} c_{i+1\sigma} + c_{i+1\sigma}^{\dagger} c_{i\sigma}) \xrightarrow{adiabatic} H(1) = H_H$$

By solving the TDSE, we can calculate state $\psi(s=1)$ from $\psi(s=0)$,

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

Gate-based simulations of quantum annealing

Time required to find the ground-state using quantum annealing?
Simulate and find out.

- We simulate quantum annealing on a gate-based quantum computer.

Steps for the simulation of quantum annealing:

1. Transform fermionic Hamiltonian to qubit Hamiltonian
2. Construct circuit for preparing initial state $\psi(s = 0)$
3. Prepare circuit for time evolution to $\psi(s = 1)$
4. Calculate the energy $\langle \psi | H_H | \psi \rangle$

$L =$ lattice size

Gate-based simulations of quantum annealing

Jordan-Wigner transformation

- We need to map the fermionic operators to qubit operators
- JW transformation:

$$c_i^\dagger \rightarrow \frac{1}{2} Z_1 \ldots Z_{i-1} (X_i - iY_i)$$

$$c_i \rightarrow \frac{1}{2} Z_1 \ldots Z_{i-1} (X_i + iY_i),$$

- Using this, the annealing Hamiltonian transforms into,

$$H(s) = -\frac{t_H}{2} \sum_{\substack{i=1 \\ i \neq L}}^{2L-1} (X_i X_{i+1} + Y_i Y_{i+1}) + \frac{sU}{4} \sum_{i=1}^{L} (I - Z_i)(I - Z_{i+L})$$

$L =$ lattice size

Gate-based simulations of quantum annealing

Initial-state preparation

Ground-state of $H(0) \rightarrow |\psi(0)\rangle = c^\dagger_{k_1\uparrow} c^\dagger_{k_2\uparrow} \ldots c^\dagger_{k_{N_\uparrow}\uparrow} \ldots c^\dagger_{k_{N_\downarrow}\downarrow} |0\rangle$

where $c^\dagger_{k\sigma} = \sqrt{\frac{2}{L+1}} \sum_{j=1}^{L} \sin(kj) c^\dagger_{j\sigma}, \quad k = \frac{m\pi}{L+1}$ with $m = 1,2,\ldots,L.$

$\downarrow$

$$\begin{pmatrix} c^\dagger_{k_1} \\ \cdot \\ c^\dagger_{k_N} \end{pmatrix} = Q \begin{pmatrix} c^\dagger_{i_1} \\ \cdot \\ c^\dagger_{i_N} \end{pmatrix}$$

It turns out: $Q = G_1 G_2 \ldots G_{n_g}$

where $G_a(\theta) = \begin{pmatrix} \cos(\theta_a) & -\sin(\theta_a) \\ \sin(\theta_a) & \cos(\theta_a) \end{pmatrix}$

Zhang Jiang et al., PRA 9, 044036 (2018)

$L =$ lattice size

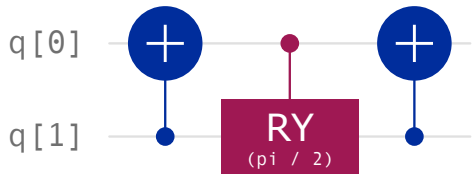
Gate-based simulations of quantum annealing

Initial-state preparation

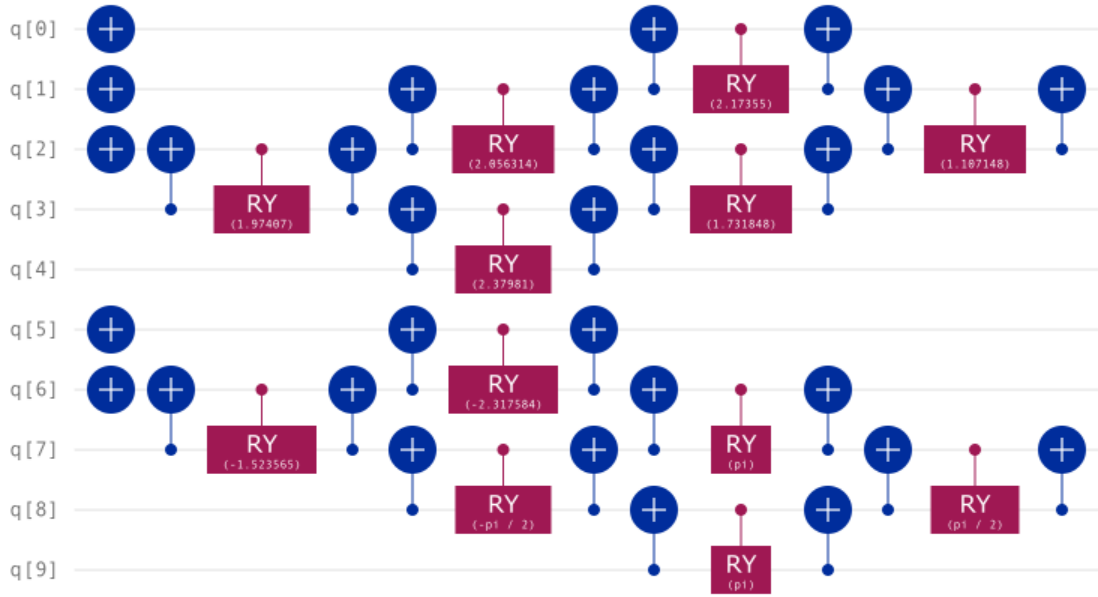
Given Q, the sequence of Givens rotations can be calculated in an efficient way.

A circuit that implements a Givens rotation on neighbouring sites

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



$$n_g = O(L^2)$$
Depth $= L - 1$
for $2N_\downarrow = N = L$



Full circuit to prepare initial-state for a system with $L = N = 5, N_\downarrow = 2 \rightarrow$

Zhang Jiang et al., PRA 9, 044036 (2018)

$L =$ lattice size

Gate-based simulations of quantum annealing

Suzuki-Trotter product-formula algorithm

The final state after quantum annealing is given by the solution to the TDSE,

$$|\psi(T_A)\rangle = U(T_A,0)\,|\psi(0)\rangle \text{ under } H(s) \text{ with } s = \frac{t}{T_A}$$

We use the second order product-formula algorithm

$$U(T_A,0) \approx \prod_{n=1}^{n=\frac{T_A}{\tau}} \left(e^{i\frac{tH\tau}{4}XX} e^{-i\frac{Un\tau^2}{8}ZZ} e^{i\frac{tH\tau}{2}YY} e^{-i\frac{Un\tau^2}{8}ZZ} e^{i\frac{tH\tau}{4}XX} \right)$$

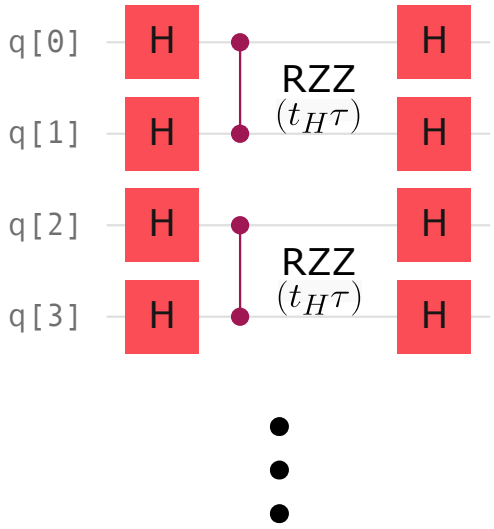
$$XX = \sum_{\substack{i=1 \\ i \neq L}}^{2L-1} X_i X_{i+1}, \qquad YY = \sum_{\substack{i=1 \\ i \neq L}}^{2L-1} Y_i Y_{i+1}, \qquad ZZ = \sum_{i=1}^{L} (I - Z_i)(I - Z_{i+L})$$

Gate-based simulations of quantum annealing

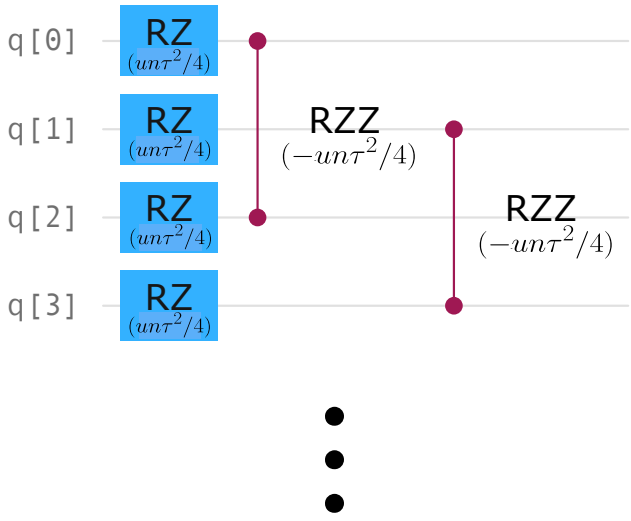
Circuits

The circuits contain sequences of only gates of the form $e^{i\frac{t_H\tau}{2}XX}$, $e^{i\frac{t_H\tau}{2}YY}$ and $e^{-i\frac{un\tau^2}{8}ZZ}$.

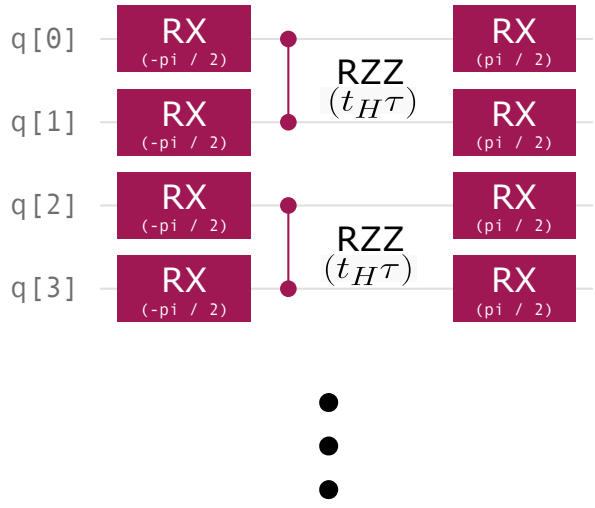
$e^{i\frac{t_H\tau}{2}XX}$



$e^{-i\frac{un\tau^2}{8}ZZ}$



$e^{i\frac{t_H\tau}{2}YY}$

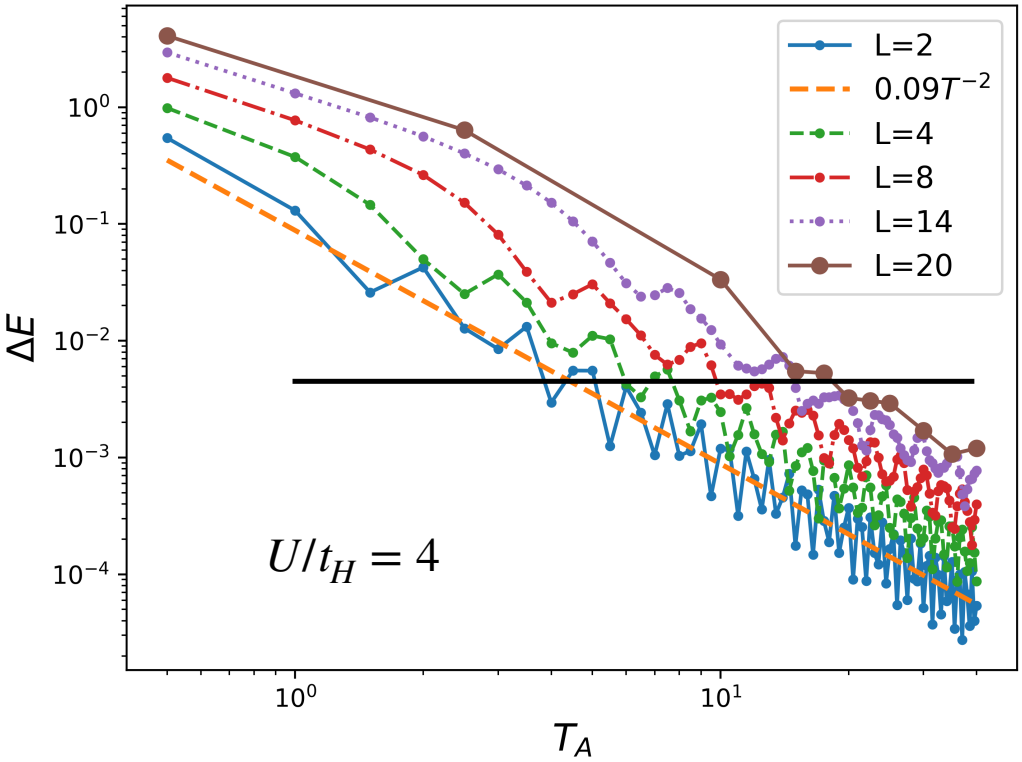


- Gates required to implement one trotter-step $\rightarrow O(L)$
- Gates required to implement complete time-evolution $\rightarrow O(L \times T_A(L))$

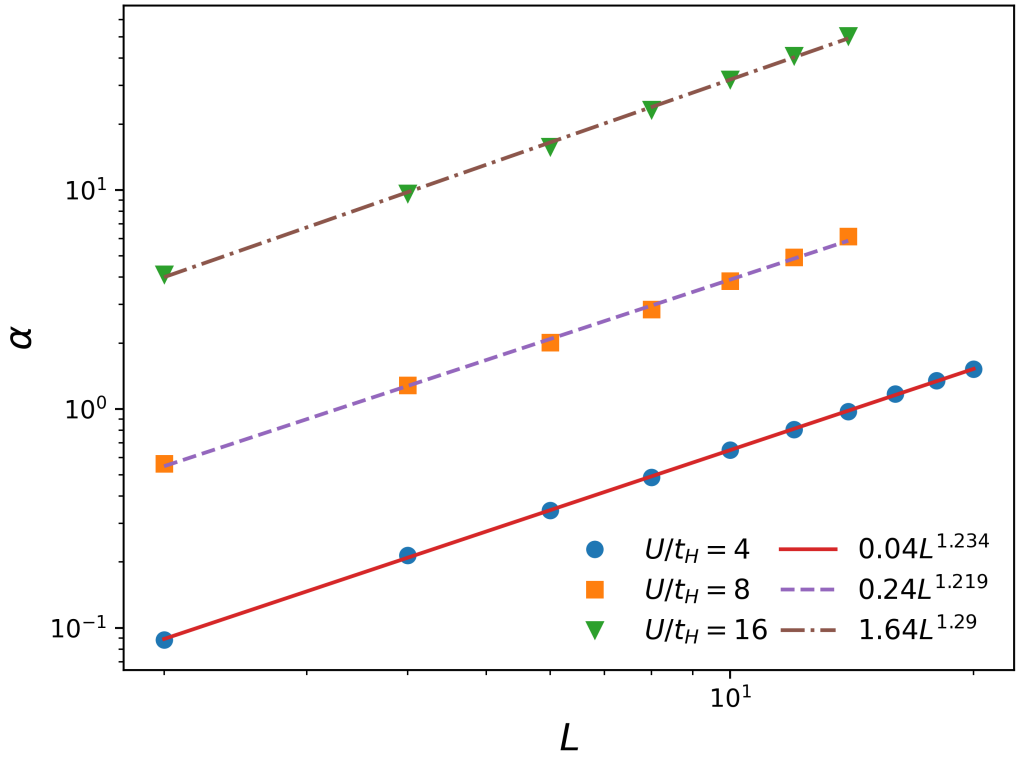
$L =$ lattice size

Results

- After constructing circuits for L up to 20 and a range of T_A, we simulate them using the high-performance Jülich Universal Quantum Computer Simulator.
- We calculate $\Delta E = \langle \psi(T_A) | H_H | \psi(T_A) \rangle - E_0$.



ΔE^*



for a certain value of the energy residue $\epsilon(L)$, when $\Delta E \leq \epsilon(L)$

$$\Delta E \approx \frac{\alpha(L)}{T_A^2} \quad \rightarrow$$

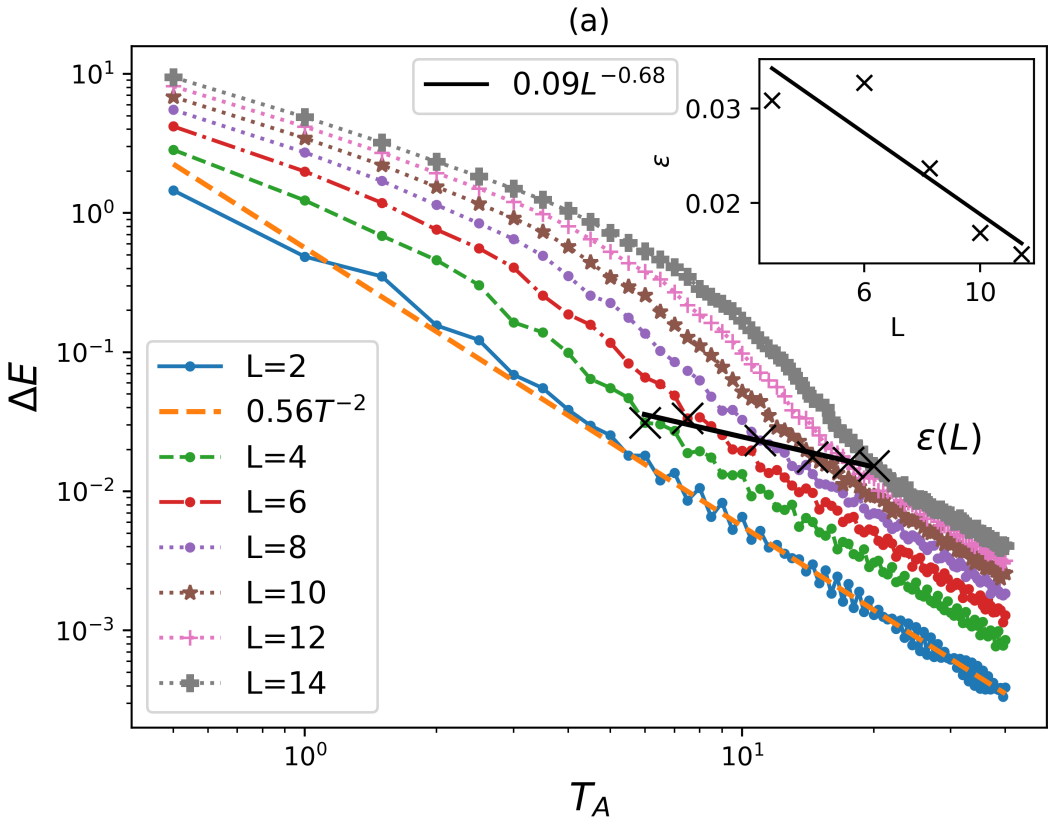
For a desired precision $\Delta E^* \approx \epsilon(L^*)$, if $L < L^*$

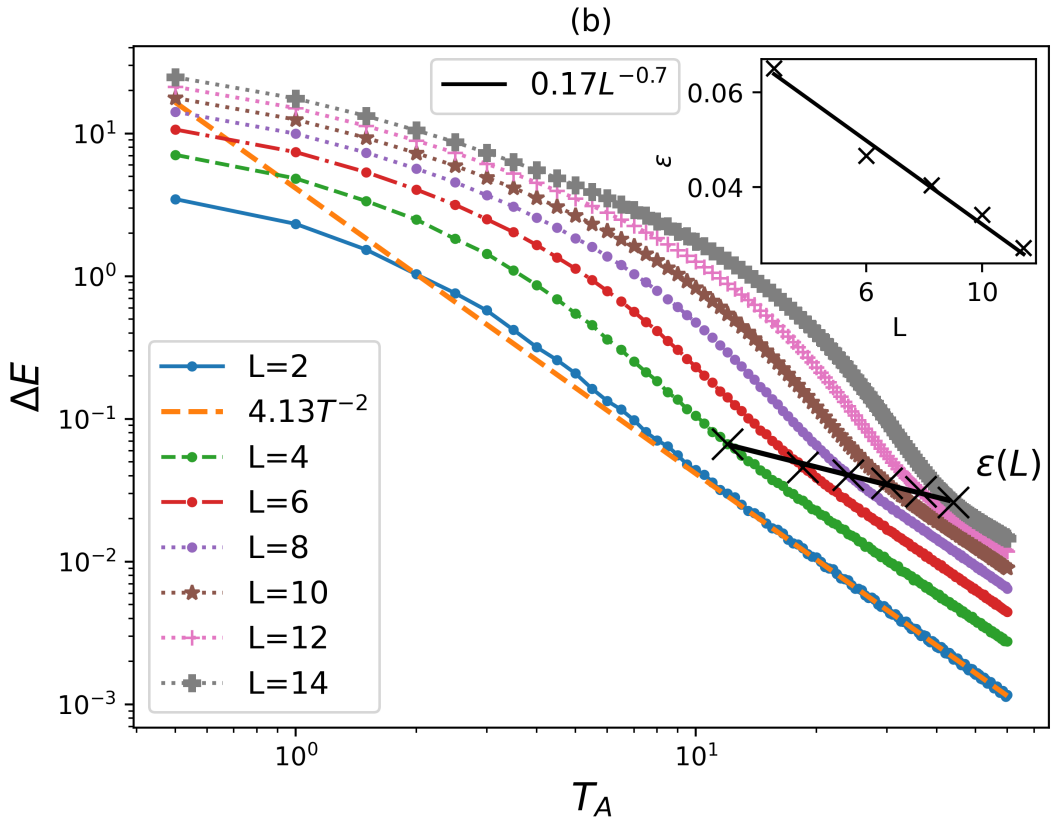
$$T_A \propto \frac{L^{0.62}}{\sqrt{\Delta E^*}}$$

$\leftarrow \quad \alpha(L) \propto L^{1.238}$

L = lattice size

Results





For $L > L^*$, where $\Delta E^* > \epsilon(L^*)$,

$$T_A < T_A' \approx \sqrt{\frac{\alpha(L)}{\epsilon(L)}}$$

$$\epsilon(L) \sim L^{-0.7}$$

$$\rightarrow \quad T_A < T_A' \propto L^{0.995}$$

Comments on the adiabatic theorem

- From the adiabatic theorem, we have a bound for the transition probability:

$$1 - \|\langle E_0 | \psi(T_A)\rangle\|^2 \leq \frac{1}{T_A^2}\left(\frac{\|\dot{H}(0)\|}{\Delta^2(0)} + \frac{\|\dot{H}(1)\|}{\Delta^2(1)} + \int_0^1 \left(7\frac{\|\dot{H}\|^2}{\Delta(s)^3} + \frac{\|\ddot{H}\|}{\Delta(s)^2}\right) ds\right)^2$$

- Large $T_A \to T_A^{-2}$ behaviour of the transition probability.

- If $\dot{H}(0) = \dot{H}(1) = 0$, the leading order term in the bound changes to T_A^{-4}.

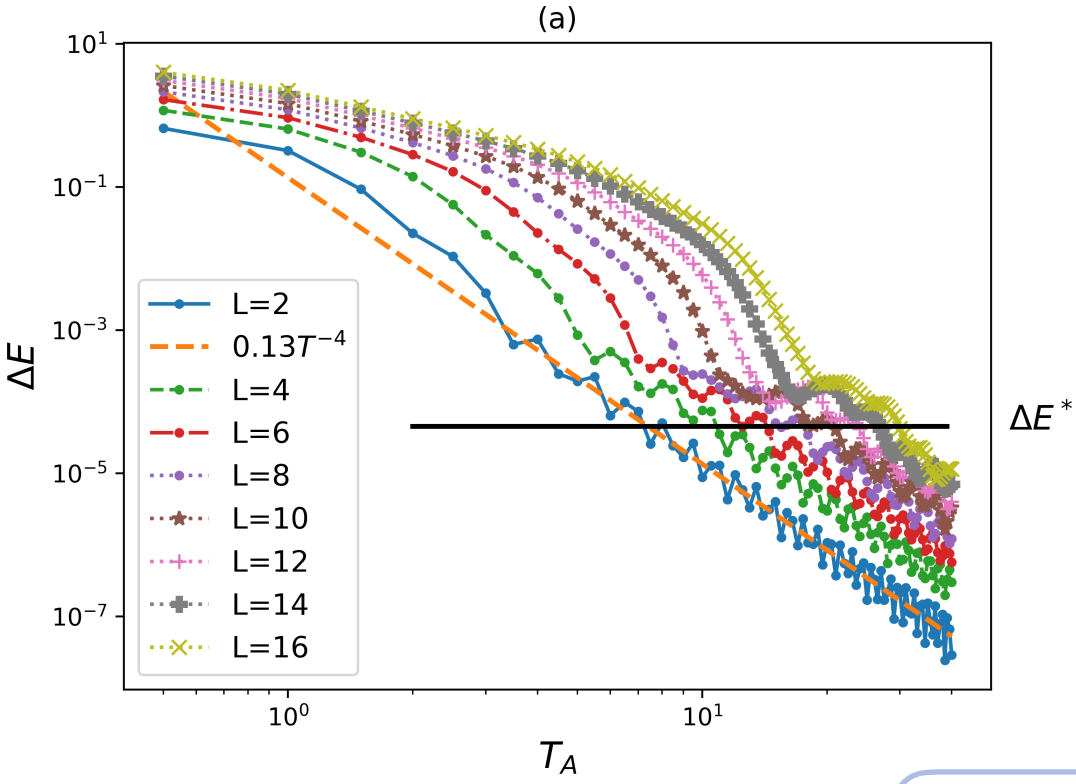
Sabine Jansen et al., *J. Math. Phys.* 48, 102111 (2007)

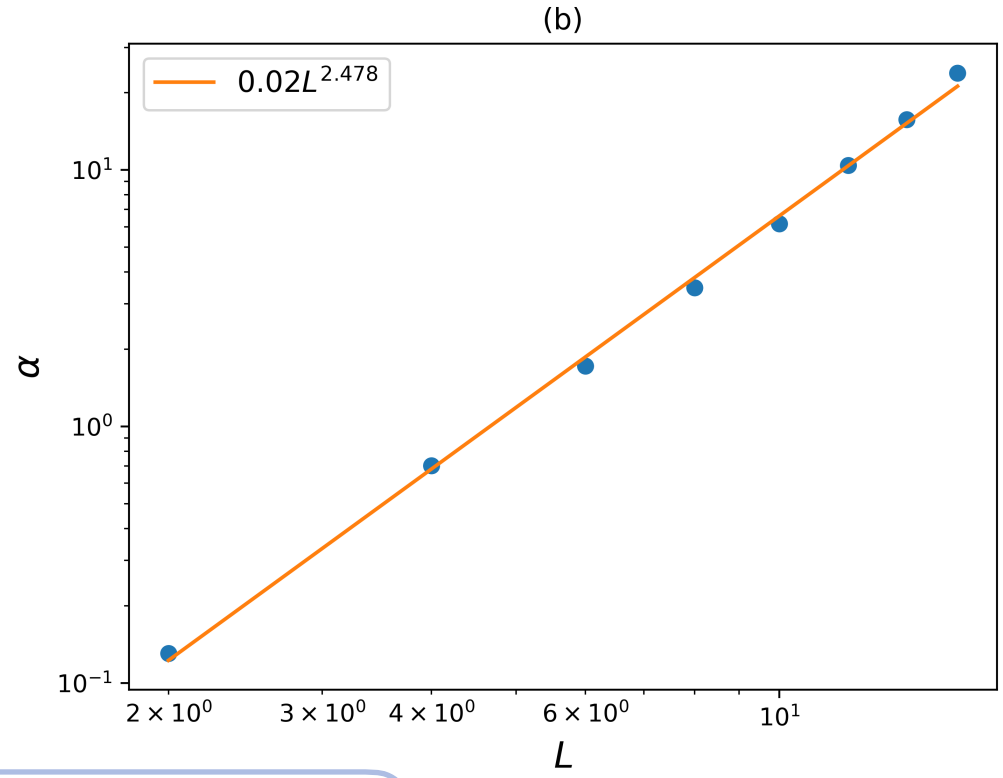
L = lattice size

Results

Sinusoidal schedule

$$H(s) = -t_H \sum_{\langle i,j\rangle,\sigma}^{L} (c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) + \frac{\sin(\pi s - \pi/2) + 1}{2} u \sum_{i}^{L} n_{i\uparrow} n_{i\downarrow}$$





When $\Delta E \leq \epsilon(L)$

$$\Delta E \approx \frac{\alpha(L)}{T_A^2} \quad \rightarrow$$

For a desired precision
$\Delta E^* \approx \epsilon(L^*)$, if $L < L^*$

$$T_A \propto \frac{L^{0.62}}{\sqrt[4]{\Delta E^*}}$$

$\leftarrow \quad \alpha(L) \propto L^{2.487}$

Summary

- We discussed classical algorithms to find the ground state of the one-dimensional Hubbard model.
- We demonstrated how to implement the algorithm of quantum annealing on a gate-based quantum computer detailing the involved steps for the problem under consideration.
- Concluding with the analysis of the simulation results, we showed that the time required to find a reasonable estimate of the ground state of the one-dimensional Hubbard model scales at most linearly using quantum annealing.

Thank you very much!