



QUANTUM SPEED-UP USING QUANTUM ANNEALING TO SOLVE THE 1D FERMI-HUBBARD MODEL

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The Hubbard model

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

$$H_H = -t_H \sum_{i=1}^{L-1} \sum_{\sigma=\uparrow, \downarrow} (c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+1\sigma}^\dagger c_{i\sigma}) + u \sum_i^L n_{i\uparrow} n_{i\downarrow}$$

- 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?

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
$$= \binom{N}{N_{\downarrow}}^2.$$
- $O(D^3)$ time to find the ground-state $\rightarrow$ **exponential** for $2N_{\downarrow} = N = L$.

Lanczos algorithm

- Exact calculation of the low lying eigenstates and eigenvalues by repeated application of $H_H |\psi\rangle$.
- $O(L \times D)$ time to find ground-state $\rightarrow$ **exponential** for $2N_{\downarrow} = N = L$.

Classical algorithms

Bethe-ansatz equations

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

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

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

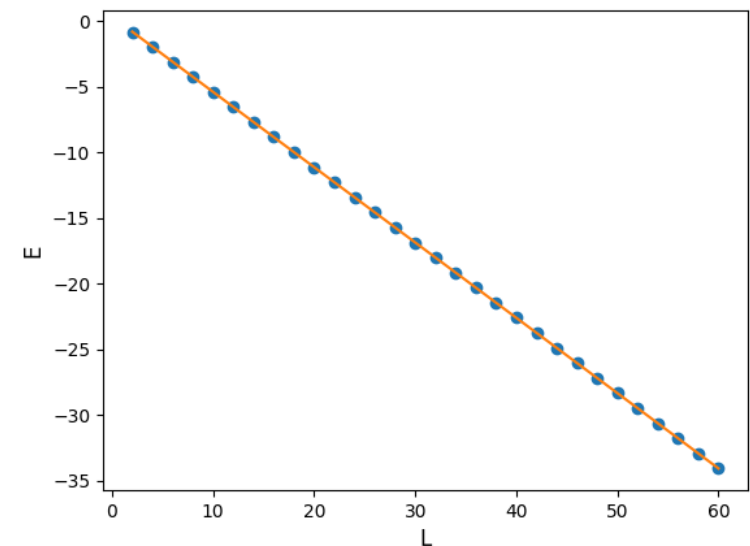
$$\sum_{b=\pm 1} \sum_{l=1}^N \phi(2b \sin k_l + 2\lambda_r) = -2\pi J_r + \sum_{b=\pm 1} \sum_{s \neq r}^{N_\downarrow} \phi(\lambda_r + b\lambda_s)$$

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

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

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

- No known analytical method to solve
- Root finding $\rightarrow$ **cubic time in L**



Quantum annealing

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

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

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

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

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

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

For a faithful 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 Schrödinger evolution to $\psi(s = 1)$

Gate-based simulations of quantum annealing

Jordan-Wigner transformation

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

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

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

- Using this, the annealing Hamiltonian transforms into,

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

Gate-based simulations of quantum annealing

Initial-state preparation

Ground-state of $H(0) \rightarrow |\psi(0)\rangle = c_{k_1\uparrow}^\dagger c_{k_2\uparrow}^\dagger \dots c_{k_{N\uparrow}\uparrow}^\dagger \dots c_{k_{N\downarrow}\downarrow}^\dagger |0\rangle$

where $c_{k\sigma}^\dagger = \sqrt{\frac{2}{L+1}} \sum_{j=1}^L \sin(kj) c_{j\sigma}^\dagger$, $k = \frac{m\pi}{L+1}$ with $m = 1, 2, \dots, L$.

↓

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

It turns out: $Q = G_1 G_2 \dots G_{n_g}$
 where $G_a(\theta) = \begin{pmatrix} \cos(\theta_a) & -\sin(\theta_a) \\ \sin(\theta_a) & \cos(\theta_a) \end{pmatrix}$

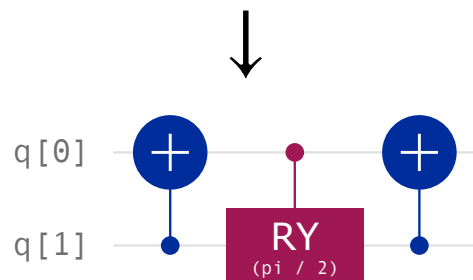
Gate-based simulations of quantum annealing

Initial-state preparation

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

A circuit that implements a Givens rotation on neighbouring sites

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

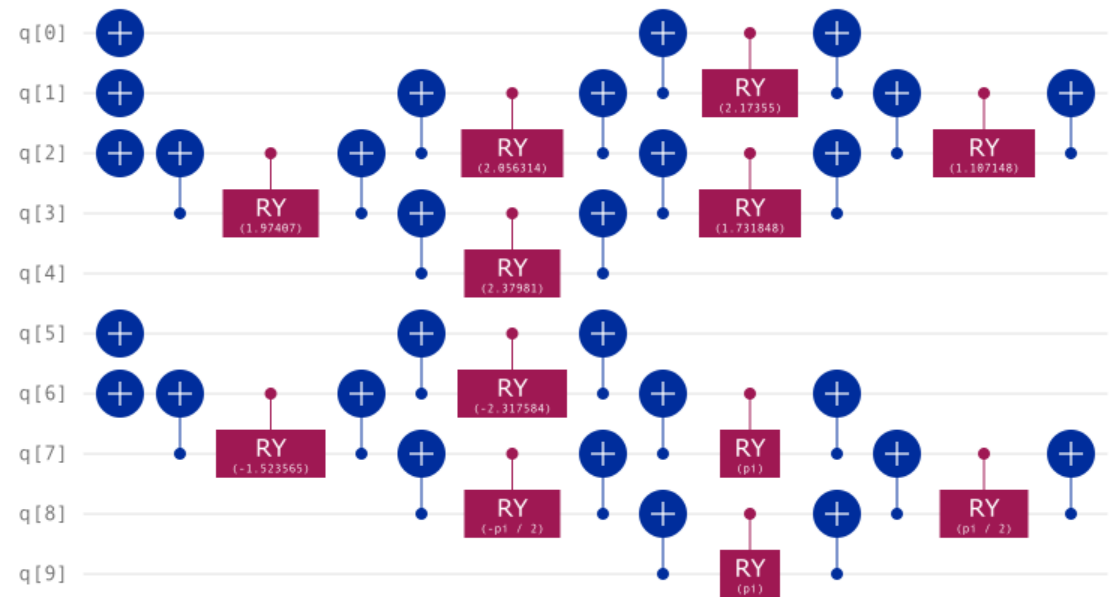


Full circuit to prepare initial-state for a system with $L = N = 5, N_\downarrow = 2 \rightarrow$

$$n_g = O(L^2)$$

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

for $2N_\downarrow = N = L$



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

Gate-based simulations of quantum annealing

Suzuki-Trotter product-formula algorithm

Quantum annealing is nothing but Schrödinger dynamics. The final state after quantum annealing would be

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

With second order product-formula approximation

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

where

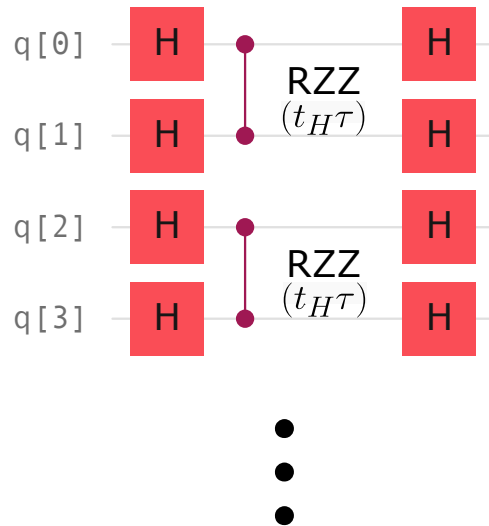
$$XX = \sum_{\substack{i=1 \\ i \neq L}}^{2L-1} X_i X_{i+1}, \quad YY = \sum_{\substack{i=1 \\ i \neq L}}^{2L-1} Y_i Y_{i+1}, \quad ZZ = \sum_{i=1}^L (I - Z_i)(I - Z_{i+L})$$

Gate-based simulations of quantum annealing

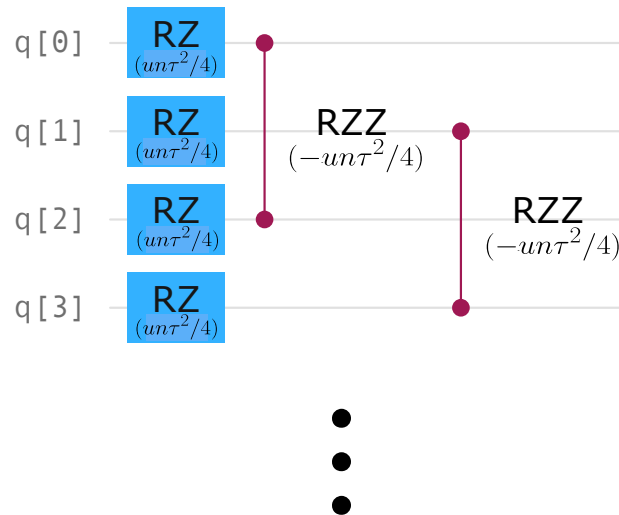
Circuits

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

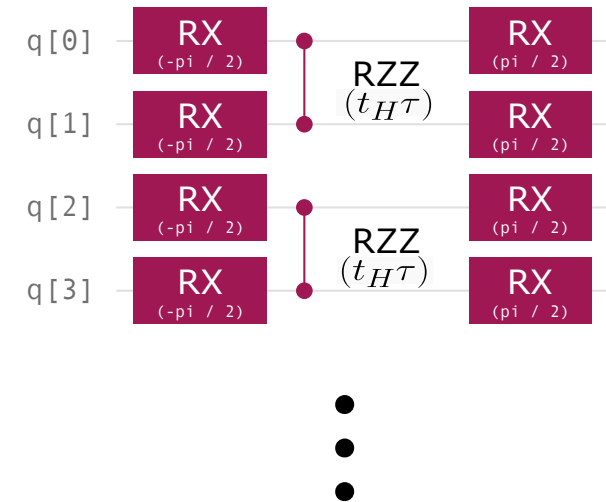
$$e^{i\frac{t_H\tau}{2}}XX$$



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



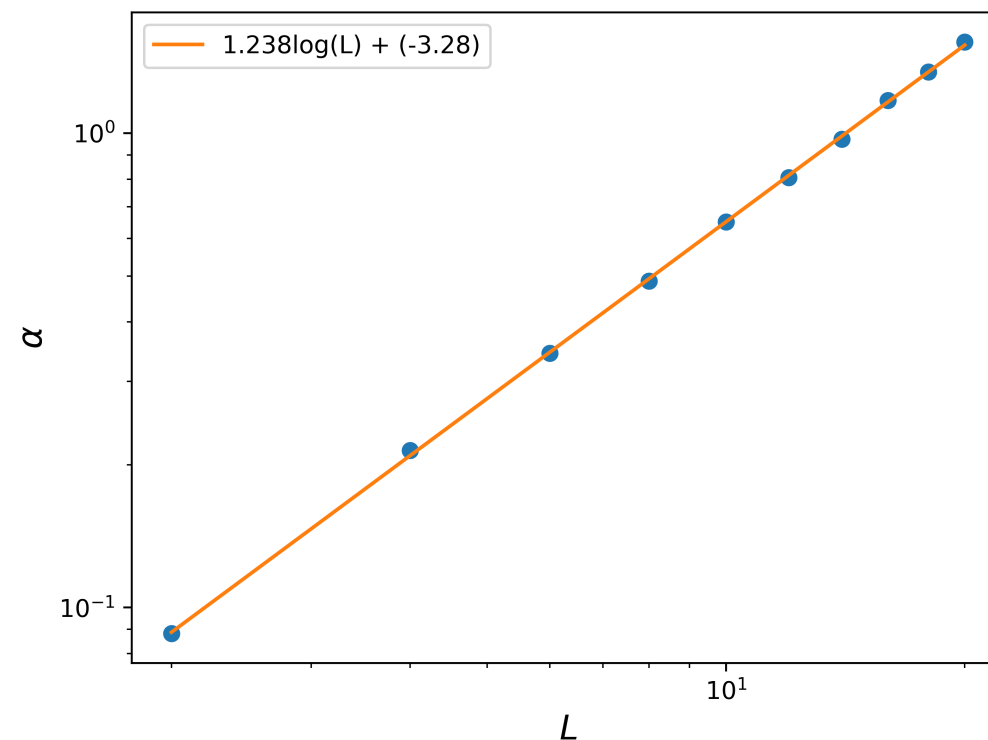
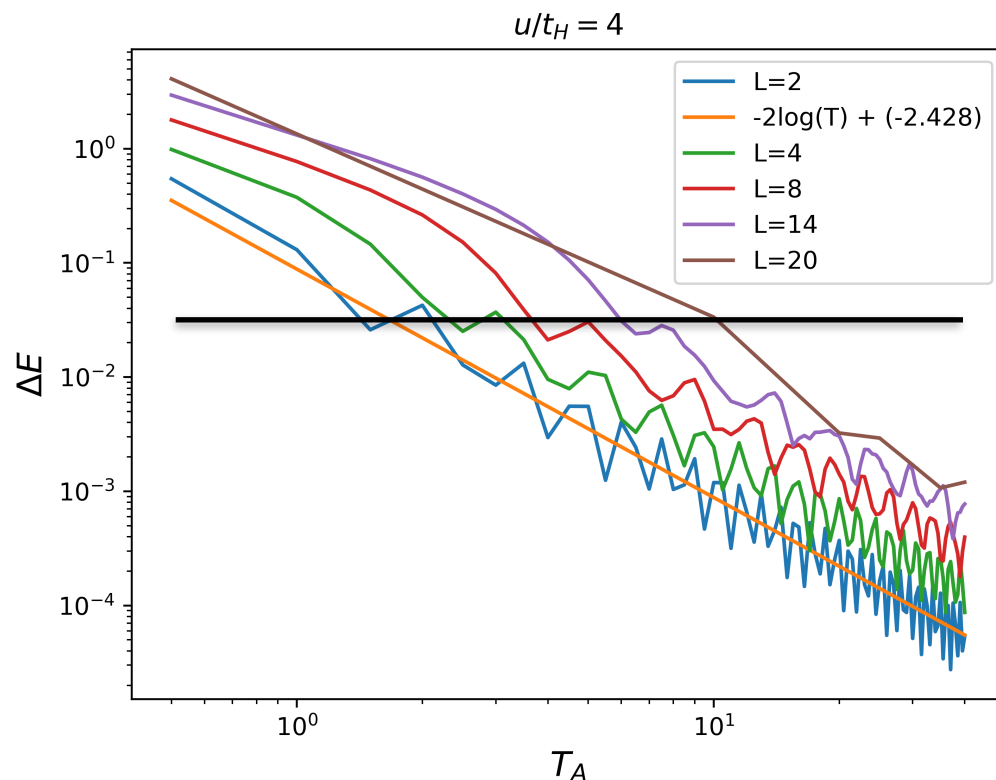
$$e^{i\frac{t_H\tau}{2}}YY$$



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

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 $\Delta E = \langle \psi(T_A) | H_H | \psi(T_A) \rangle - E_0$.



$$\Delta E = \frac{\alpha(L)}{T_A^2}$$

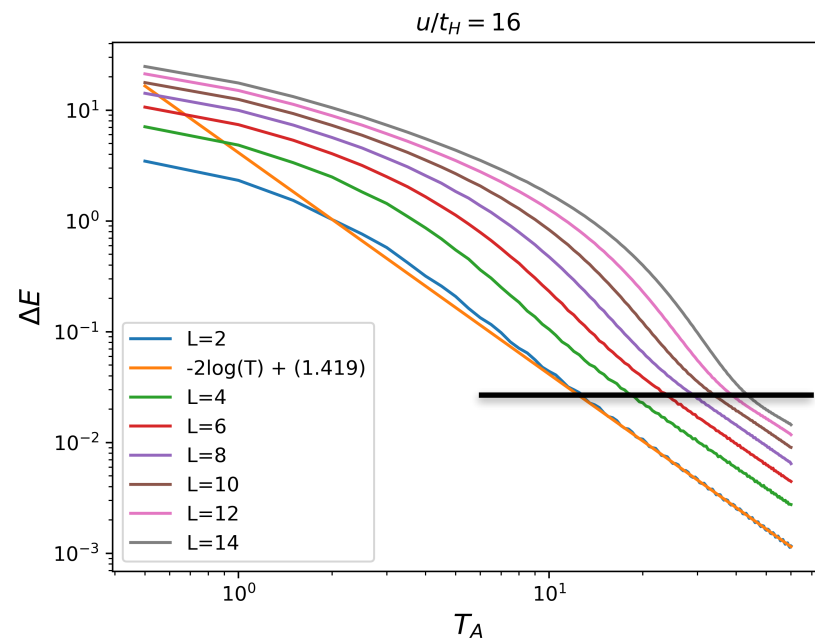
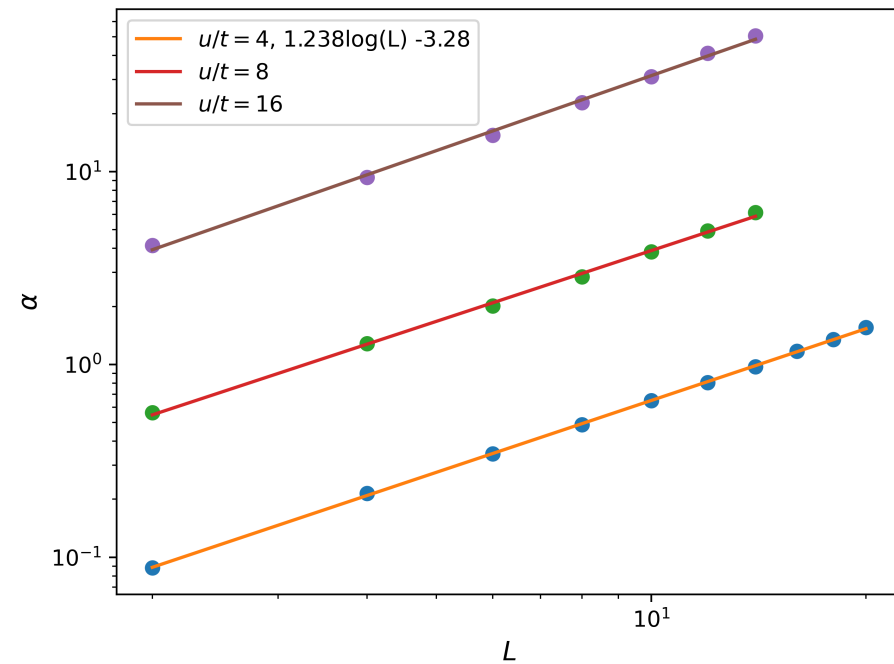
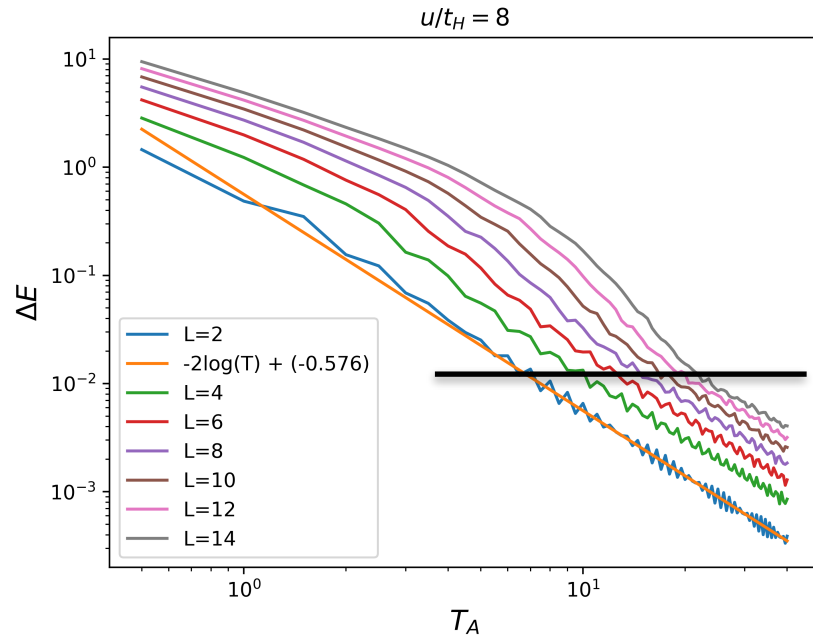
→

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

←

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

Results



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

↓

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

$$\Delta E = \frac{\alpha(L)}{T_A^2}$$



Comments on the adiabatic theorem

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

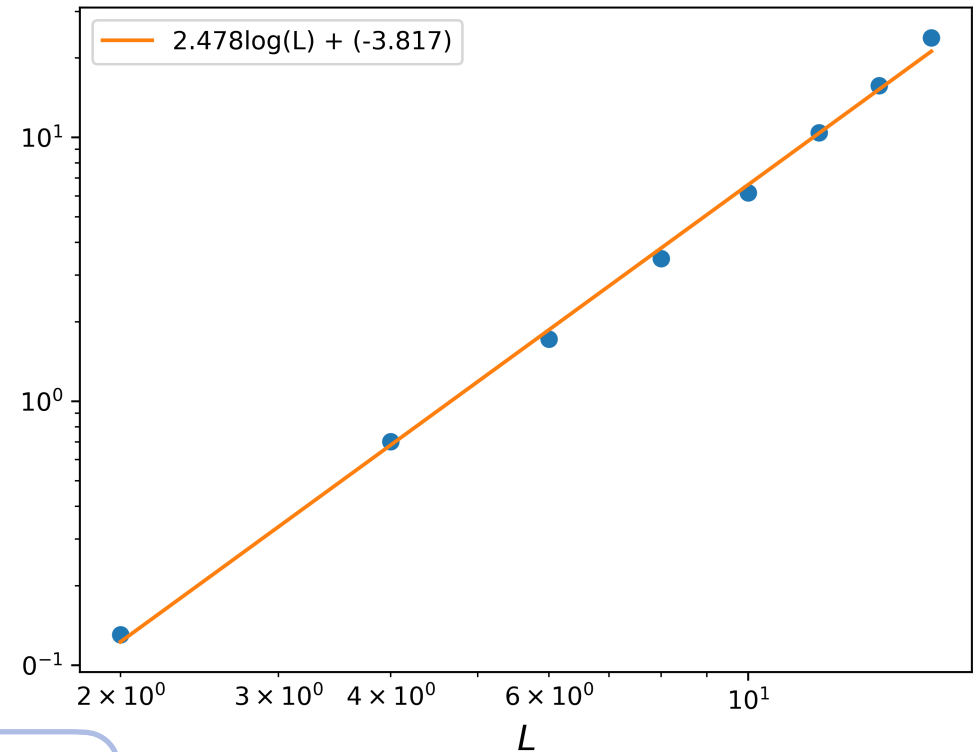
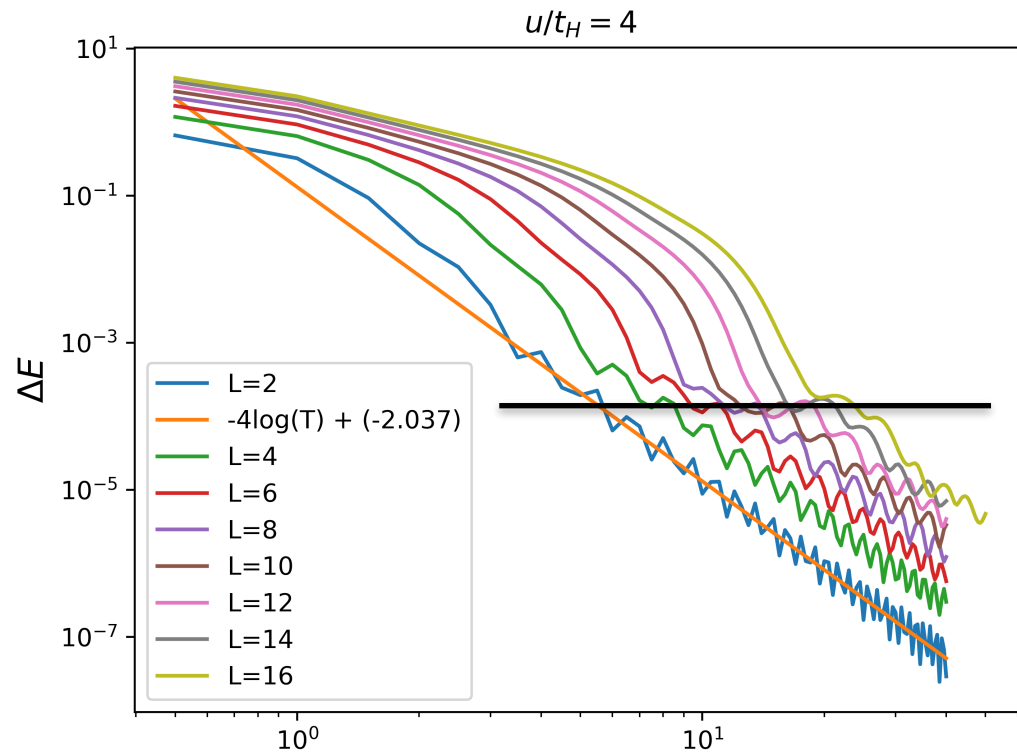
$$1 - \|\langle E_0 | \psi(T_A) \rangle\|^2 \leq \frac{1}{T_A^2} \left(\frac{\|\dot{H}(0)\|}{\Delta^2(0)} + \frac{\|\dot{H}(1)\|}{\Delta^2(1)} + \int_0^1 \left(7 \frac{\|\dot{H}\|^2}{\Delta(s)^3} + \frac{\|\dot{H}\|}{\Delta(s)^2} \right) ds \right)^2$$

- Large $T_A \rightarrow T_A^{-2}$ 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} .

Results

Sinusoidal schedule

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



$$\Delta E = \frac{\alpha_{\sin}(L)}{T_A^4} \rightarrow T_A \propto \frac{L^{0.62}}{\sqrt[4]{\Delta E}} \leftarrow \alpha_{\sin} \propto L^{2.478}$$

Conclusions

- The time required to find a reasonable estimate of the ground-state of the 1-dimensional Hubbard model using quantum annealing scales **sub-linearly** with system size.
- This result provides evidence for a polynomial **quantum speed-up** of multiple orders over the best known classical algorithm to find the ground-state of the Fermi-Hubbard model.
- For a gate-based implementation of such a protocol, the number of gates scales like $O(L^{1.62})$.

Thank you very much!