# Flow equations on quantum circuits

Unified variational methods for quantum many-body systems

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An optimal control approach to the

# Flow equations on quantum circuits

classical simulation of

## Unified variational methods for quantum many-body systems


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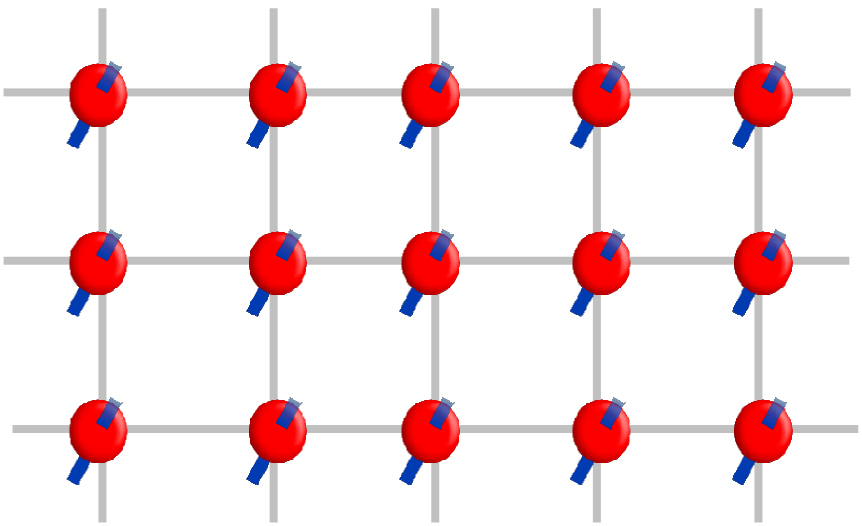
# Overview

1. Introduction – the quantum many-body problem (sort of)
2. Approximations and variational methods
   - Variational ansatzes as quantum circuits
   - Examples
3. Flow equations
   - History
   - Applications to quantum-many body problems
4. Flow equations on quantum circuits
   - Universal variational method
   - Optimal gate generators
   - Example: application to 1D Heisenberg model
5. Conclusions and TODO

# The quantum many-body problem

- Describe the ground and low-energy eigenstates of a system of $N$ interacting particles
- Generic model: particles arranged on a lattice with nearest-neighbour interactions.



$$H = \sum_{\langle j,k \rangle} K_{jk} + \sum_j H_j$$

"two-local" Hamiltonian

# “Describing” quantum systems

- *What* do we mean by a description of these low-energy states?
  - Quantitative: energy spectrum and gap, local observables, correlation functions.
  - Insight: emergence of unusual excitations or quasi-particles and their statistical properties.
- *How* do we provide these descriptions?
  - Hardly anything is exactly soluble.
  - The ground state of a system of *30* spin-½ particles (qubits) expanded in the usual basis requires *16 GB* worth of coefficients.

# Approximations and variational methods

- "Hilbert space is a big place" – for a locally interacting system with lots of symmetry only a small part should be relevant.
- In a variational method we posit a relevant subclass of states, and then try to optimize approximations within that subclass.
- e.g.
  - Mean Field Theory $|\psi\rangle = \bigotimes_{k=1}^{N} |\psi_k\rangle$
  - Density Matrix Renormalization

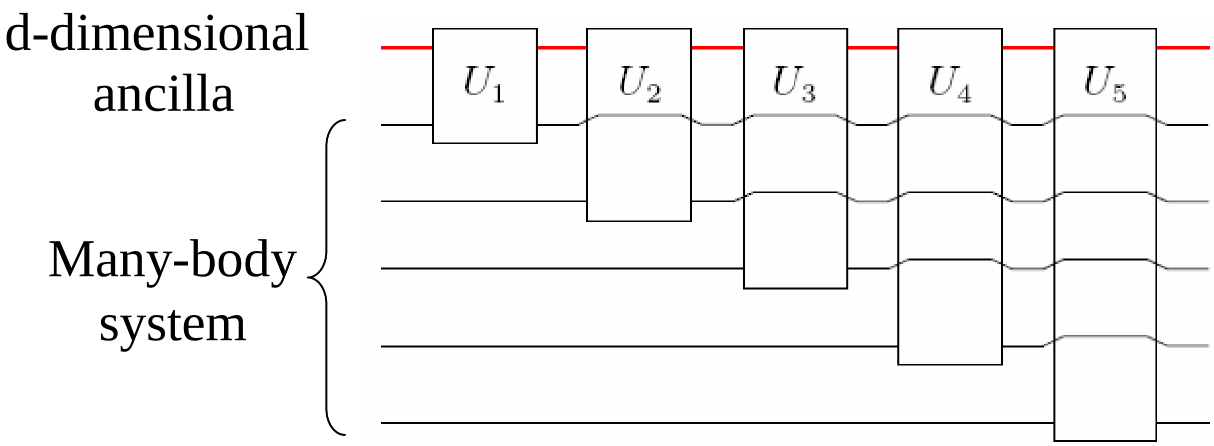
$$|\psi\rangle = \sum_{k_1,\ldots k_N} \mathrm{Tr}\left(A_1^{k_1} \cdots A_N^{k_N}\right) |k_1, \ldots, k_N\rangle$$

  - General Tensor Networks

# Variational classes as quantum circuits

- A *quantum circuit class* specifies the location of gates, any ancillary systems, and refinement parameters.
- All existing ansatz states have equivalent descriptions as quantum circuits.

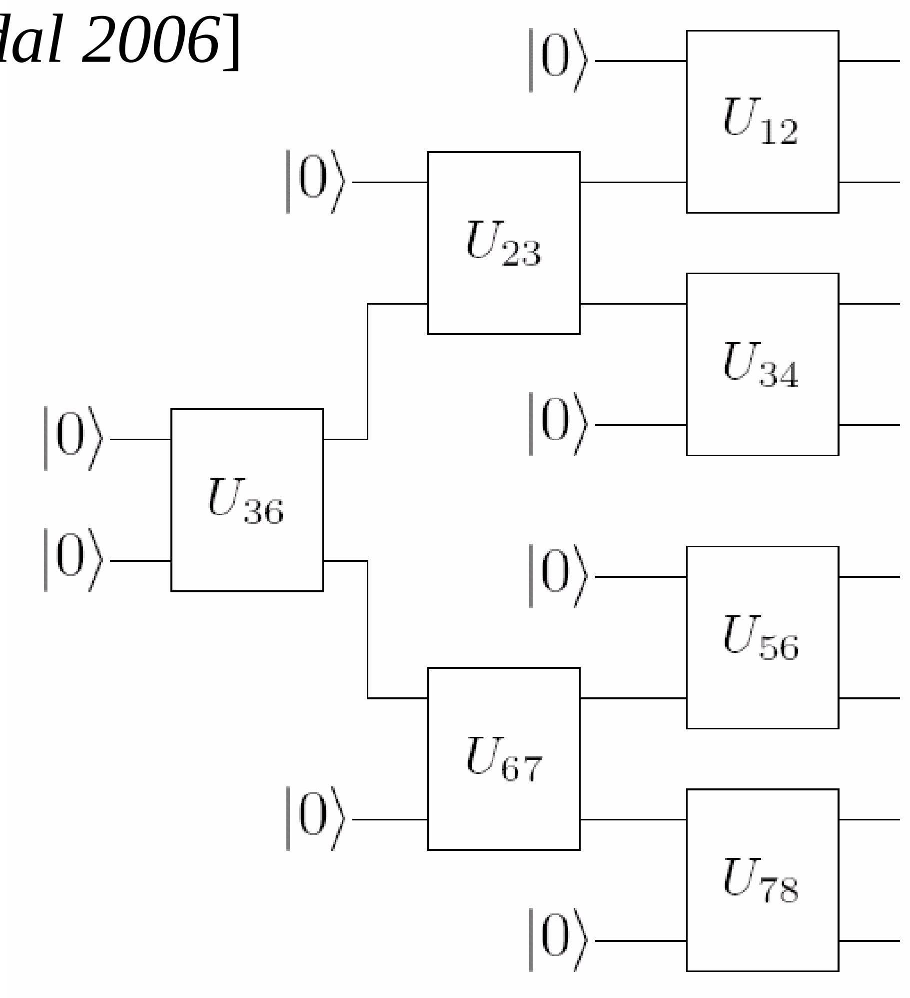
e.g. "Staircase" circuit, corresponding to matrix product states




[*Fannes, Nachtergaele, Werner 1989; Osterlund and Roemer, 1992*]

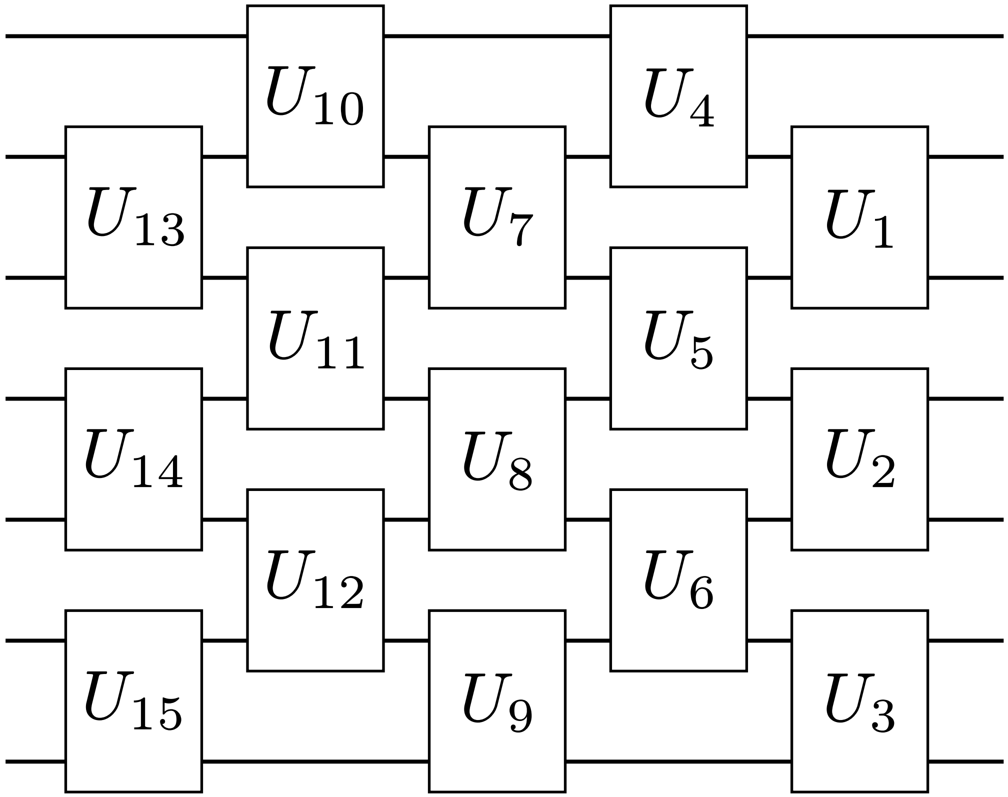
# Variational classes as quantum circuits

e.g. “MERA” circuit [*Vidal 2006*]

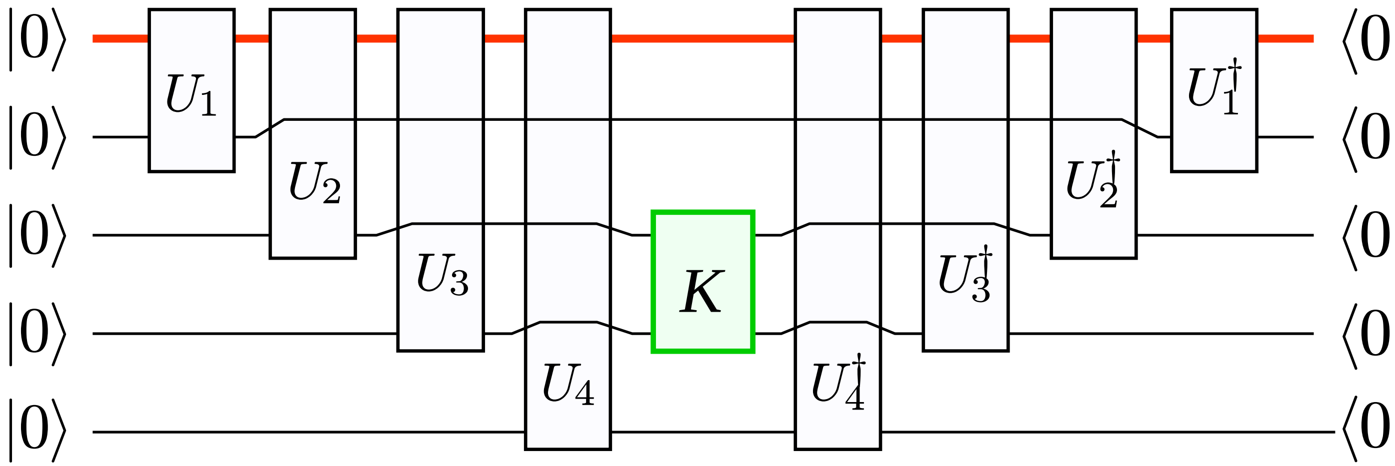


# More variational classes

e.g. *1D* Quantum cellular automata model (fixed depth)



# Desiderata: Efficient local expectations

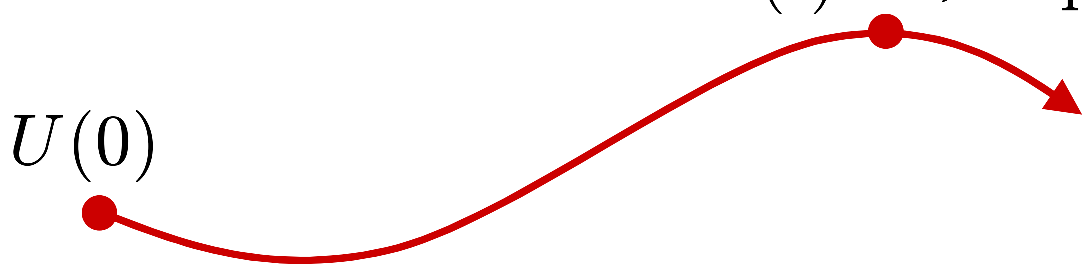



1. Cancel $U_4^\dagger U_4 = I$
2. Evaluate $U_3^\dagger K U_3$ then set $A_2 = (I \otimes \langle 0|) U_3^\dagger K U_3 (I \otimes |0\rangle)$
3. Iterate $A_{k-1} = (I \otimes \langle 0|) U_k^\dagger A_k U_k (I \otimes |0\rangle)$ until we obtain $A_0$ acting only on the auxiliary system.
4. Read out the (1,1) element.

# Flow Equations

- Analytic techniques for transforming a Hamiltonian via a continuously parameterized unitary transformation

$$U(t) = \mathcal{T} \exp\left(-i \int_0^t G(s) ds\right)$$




- For $H(t) = U(t)^\dagger H U(t)$ we find

$$\frac{dH}{dt} = -i\,[G(t), H(t)]$$

- With appropriate choice of generator *G(t)* we can obtain useful limiting forms $\lim_{t\to\infty} H(t)$

# History of Flow Equations

- Introduced independently by lots of people, in particular *Brockett*, *Glazek and Wilson*, *Wegner*.
- e.g. with $G = [H(t), N]$ we have *double-bracket* flow

$$\frac{dH}{dt} = -i\left[\left[H, N\right], H\right],$$

and if *N* is a diagonal matrix with increasing entries, then

$$\lim_{t\to\infty} H(t) = \operatorname{diag}\left(E_0, E_1, \ldots, E_n\right).$$

- Can also be used to numerically sort lists, solve linear programming problems *[Brockett 1988]*

# Flow Eqns and quantum many-body systems

- Numerical flow techniques are obviously not directly practical for $2^N \times 2^N$ Hamiltonians.
- Used as an approximate analytic method by differentiating in parameters
  - Make a clever choice for the generator *G(t)*
  - Truncate resulting system of DEs
  - Solve by whatever means necessary.
- Used to effectively diagonalize Hamiltonians, calculate correlation functions, and to take controlled expansions in strong-coupling models. [*Kehrein & Mielke*, *Wegner*]

# Flow Eqns as universal variational method

- Our approach: write variational classes for quantum many-body problems as quantum circuits, and use flow equations as a general purpose optimization method.

- *Quantum circuit class* specified by *M* gates $U_j(t)$ so the overall unitary is $U(t) = \prod_{j=1}^{M} U_j(t)$. Aim to minimize the expectation.

$$E(t) = \langle 0|U(t)^\dagger H U(t)|0\rangle$$

- Method: Calculate infinitesimal generators $G_j(t)$ individually to minimize the derivative *dE/dt*.

# Finding optimal generators

- This amounts to minimizing the real part of the quantity:

$$-i\sum_{j=1}^{M}\langle 0|U(t)^\dagger H\Big(\prod_{k=j+1}^{M}U_k(t)\Big)G_j(t)\Big(\prod_{k=1}^{j}U_k(t)\Big)|0\rangle$$

- After various rearrangements, it can be shown that the optimal generator is given by $G_j = -2(F_j + F_j^\dagger)$ with

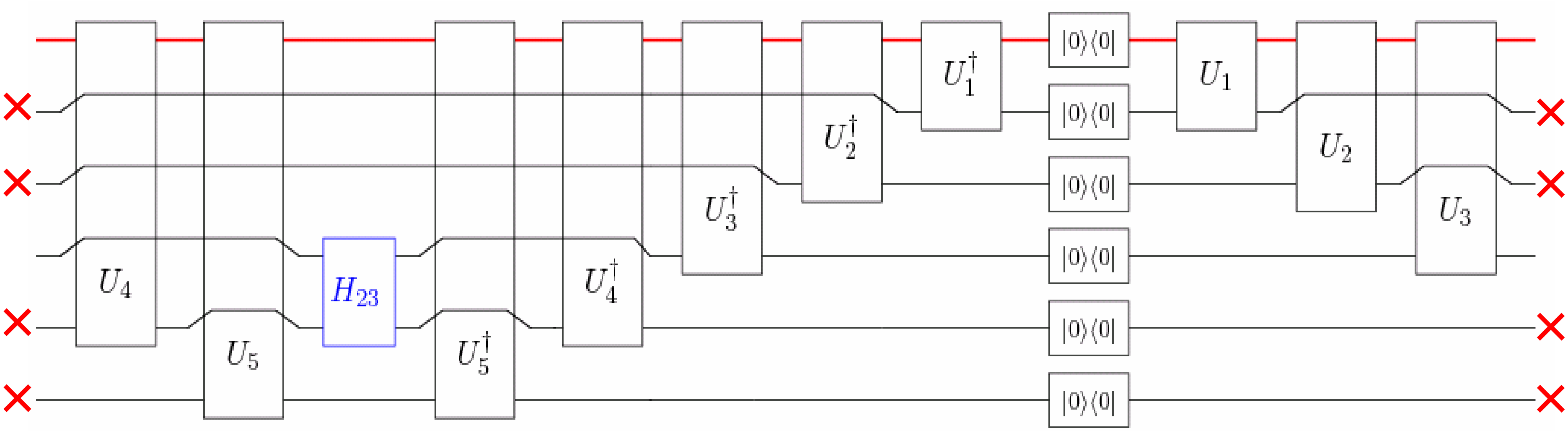
$$F_j = \mathrm{Tr}_{R_j}\left[\Big(\prod_{k=1}^{j}U_j\Big)|\mathbf{0}\rangle\langle\mathbf{0}|U^\dagger H\Big(\prod_{k=j+1}^{M}U_k\Big)\right]$$

(i.e. a partial trace over the particles not acted on by $U_j$ )

- Given $H=\sum_{\langle l,m\rangle}H_{lm}$ the circuit class must admit an efficient method of evaluating these operators.

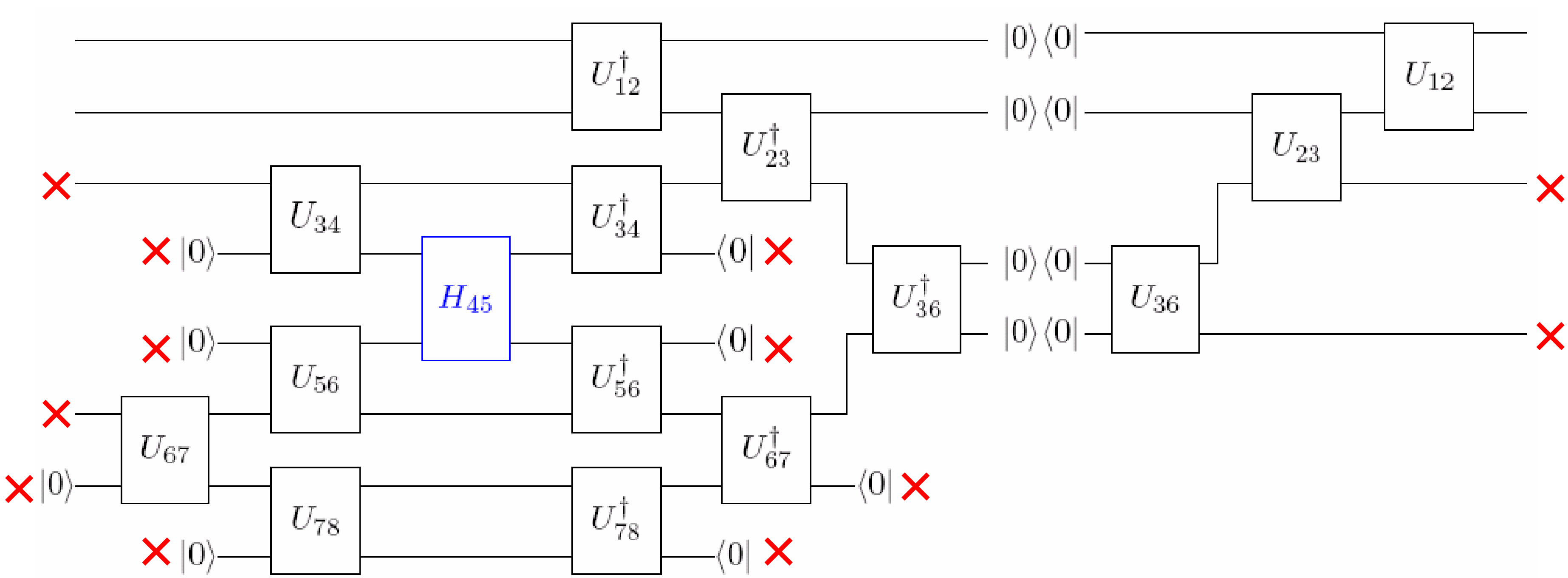
# Example (i) Contracting staircase circuits

- Contribution to the optimal generator of $U_3(t)$ due to $H_{23}$




- Can be evaluated by sequentially tracing out qubits from matrices of dimension at most $4D \times 4D$.

# Example (ii) Contracting MERA circuits



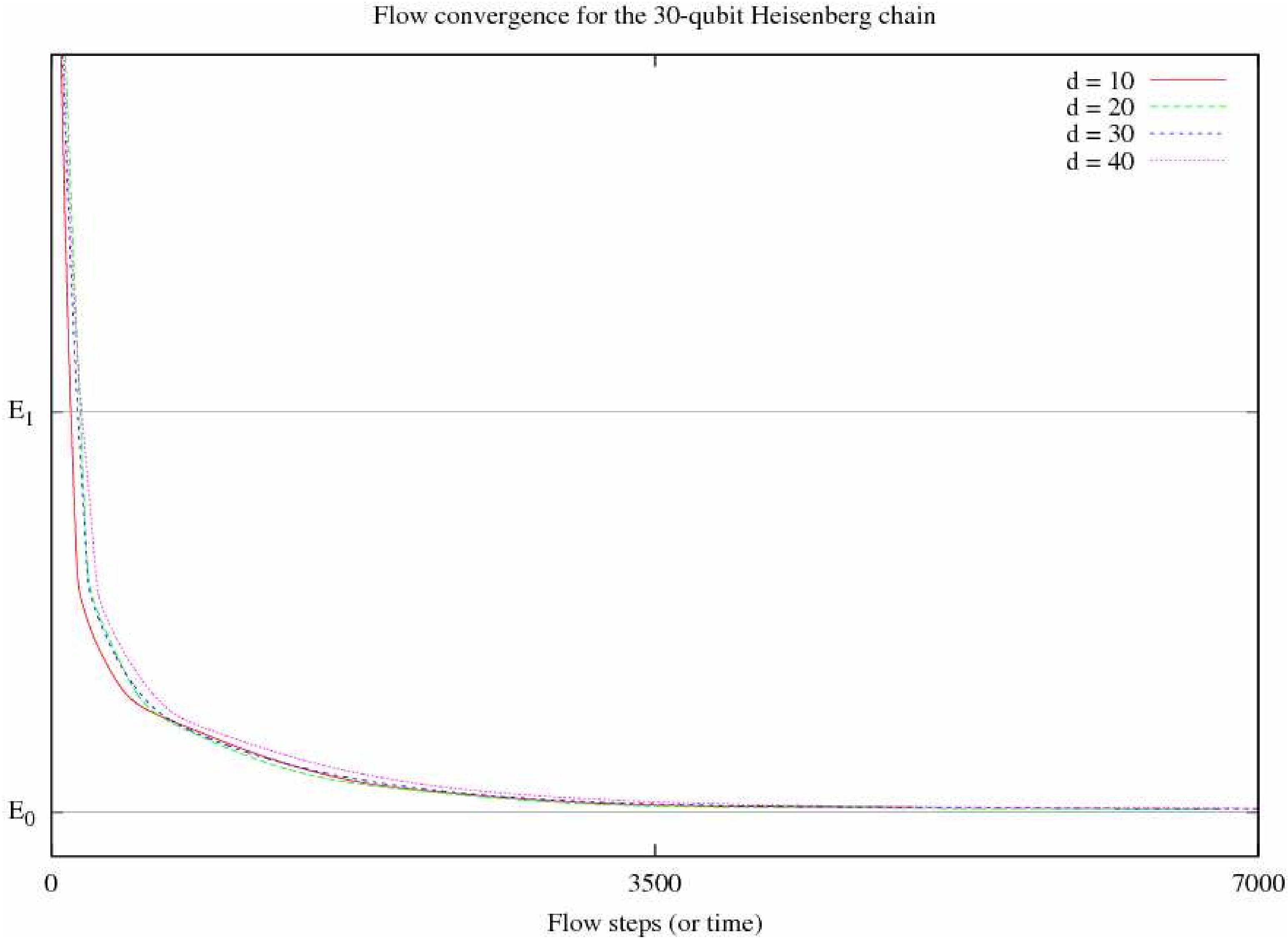

- Slightly more complicated, but same basic idea allows us to evaluate the partial trace via a sequence of smaller partial traces on (at most) $16\times16$ matrices.

# The Flow Algorithm

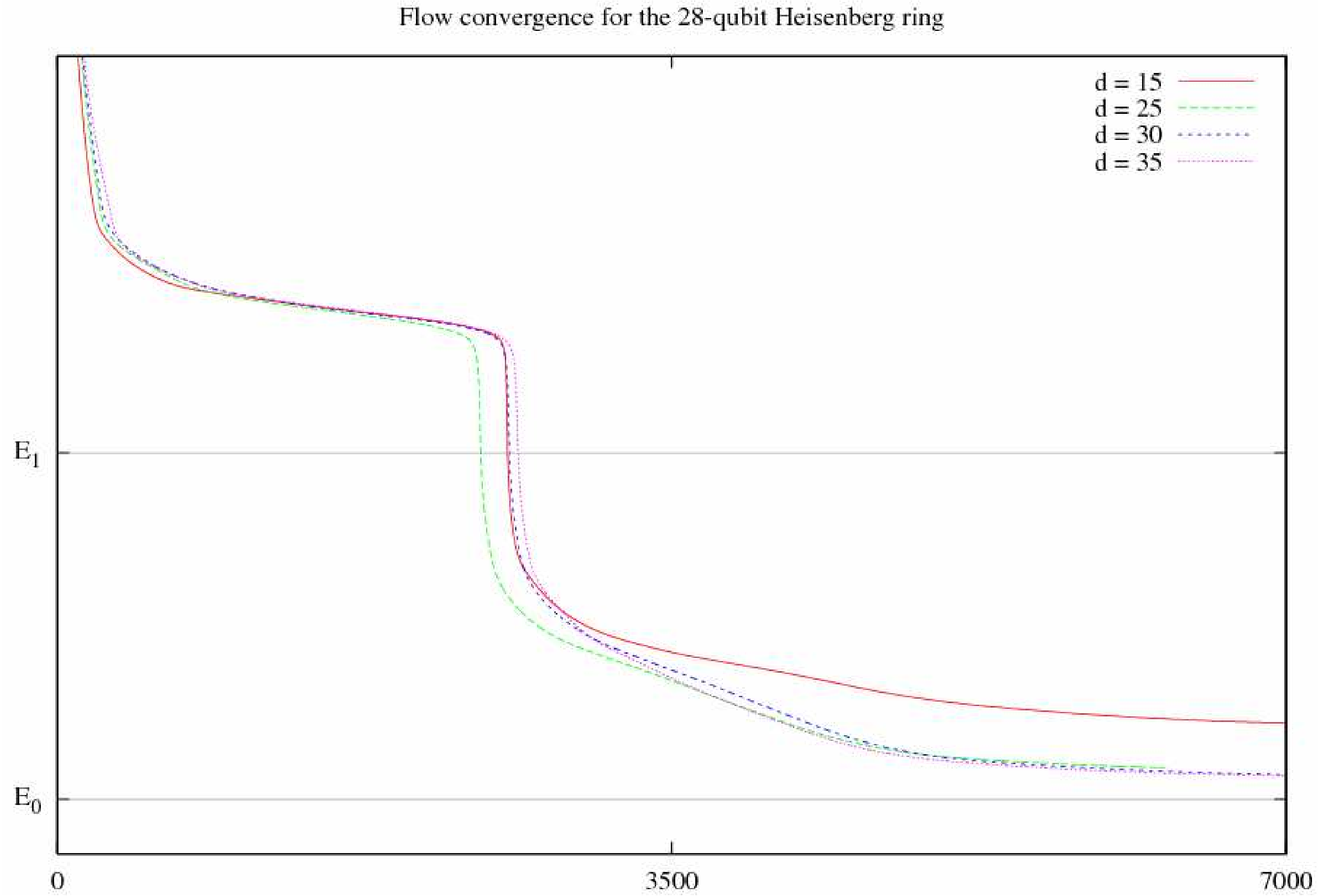
- Starting from some initial configuration of the circuit $\{U_j(0)\}$ we can implement a downhill algorithm as follows

```
Set n = 0
Initialize each U_k(0)
Set E(0) = ⟨0|U†(0) H U(0)|0⟩
do:
   for each k = 1, ..., M:
      Calculate optimal generator G_k(n)
      Calculate optimal flow strength t
      Set U_k(n+1) = exp(-i G_k(n) t) U_k(n)
   end
   n = n + 1
   Set E(n) = ⟨0|U†(n) H U(n)|0⟩
while E(n) < E(n-1)
```

# Performance with "staircase" circuits (i)



# Performance with staircase circuits (ii)



# Conclusions and TODO

1. By re-expressing ansatz states for quantum many-body systems as quantum circuits, we can use the method of flow equations as a general purpose optimization method.
2. Appeal:
   - Flexibility
   - QI has a lot to say about quantum circuits and gates
   - "The wisdom of optimal control"
3. Future work:
   - MERA version in "development"
   - 1D and 2D cellular automata circuits.