# Optimization problems on quantum computers

#### Lecture 1

Quantum optimization algorithms inspired by physics

Yassine Hamoudi

Materials: https://yassine-hamoudi.github.io/cemracs2025/

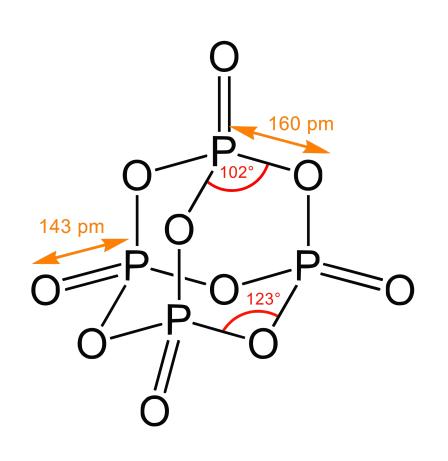
# Hackath

# Optimization is about finding elements that minimize some objectives

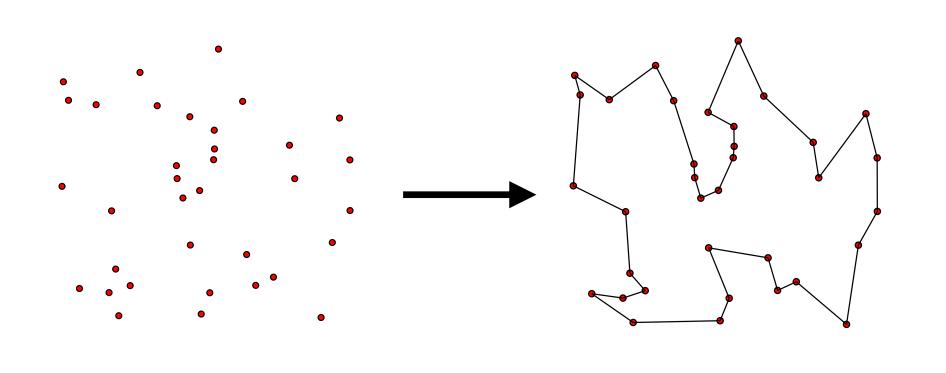
Stable configuration of a molecule

Exploration of a graph

Scheduling of concurrent tasks

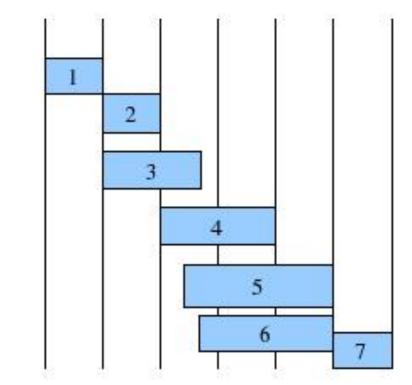


**Project: ERC EMC2** Quantum algorithms for ground state computation



**Project: L'Oréal** Genome assembly from DNA fragments Maintenance of electrical installations

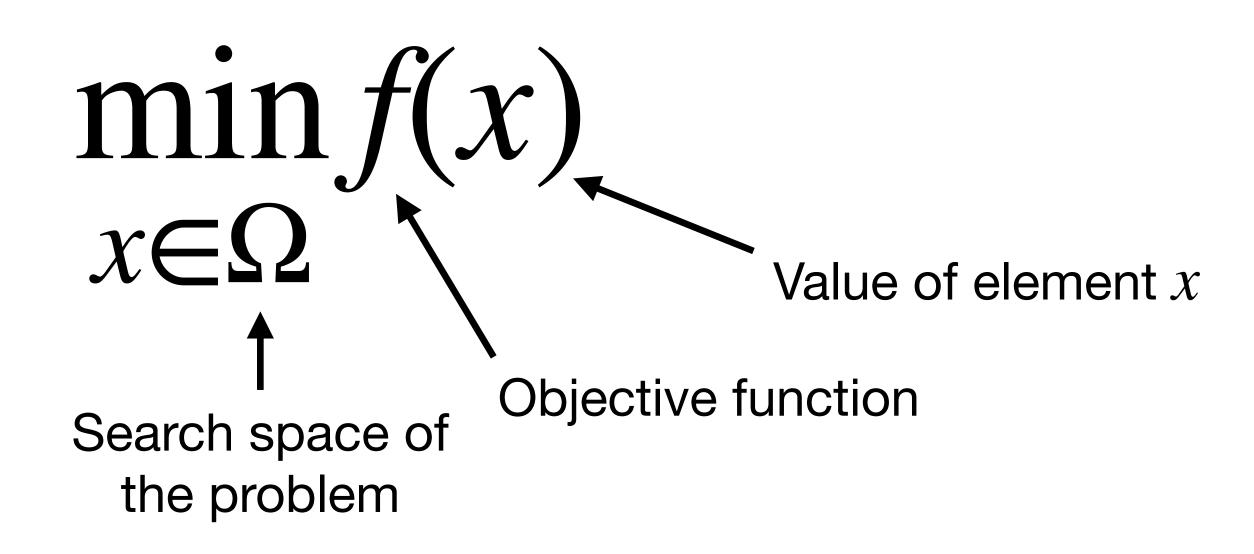
**Project: IFPEN** Route planning problems



**Project: RTE** 

**Project: La Poste** Supply of empty containers

# Optimization is about finding elements that minimize some objectives



**Example:** shortest path that connects all points

$$f\left( \checkmark \right) \leq f\left( \checkmark \right) \leq f\left( \checkmark \right)$$

f = length of a given path

$$\Omega$$
 = set of all valid paths

#### Focus of this course

How quantum computers may help in solving optimization problems?

- New types of algorithms based on the capabilities of quantum computers
- Example of optimization problems solved by such quantum algorithms
- Benefits and limitations compared to other optimization methods

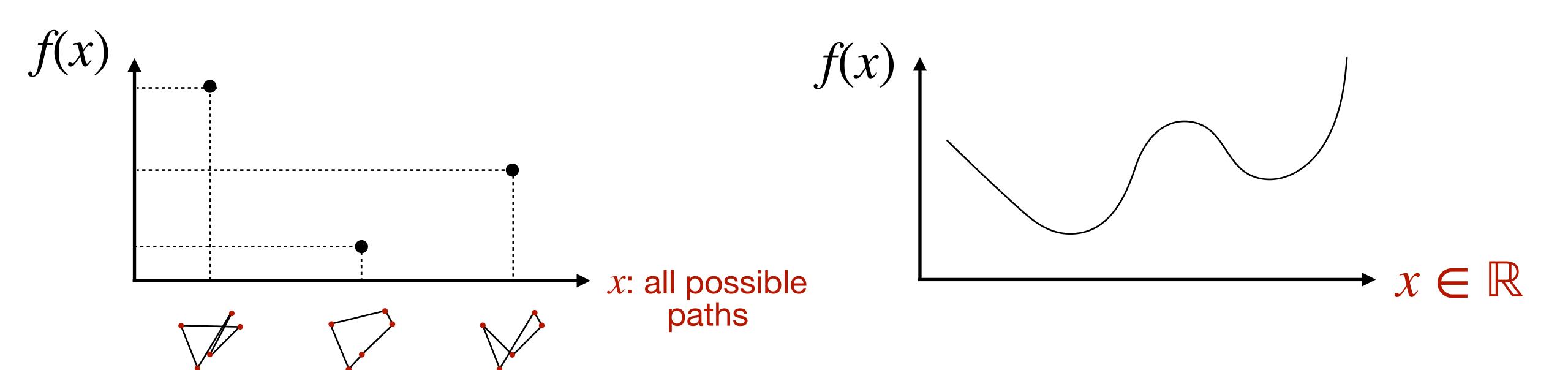
# Terminology

#### Discrete optimization

Objective function supported over a discrete set of values

#### Continuous optimization

Objective function supported over a continuous set of values



# Terminology

#### **Exact** solution

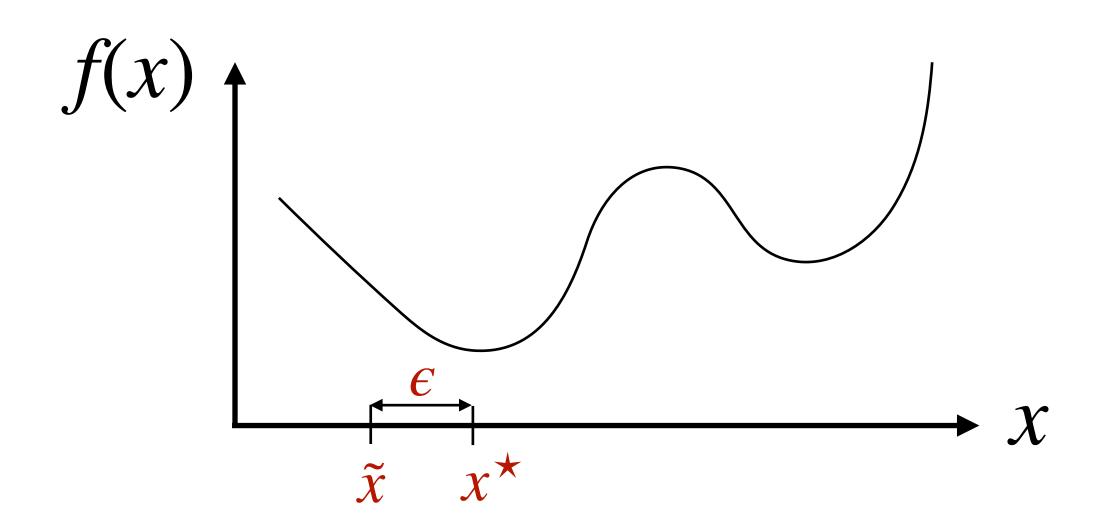
Find the minimum-value solution (or one of them if there are many)

$$\forall x, f(x^*) \leq f(x)$$

#### Approximate solution

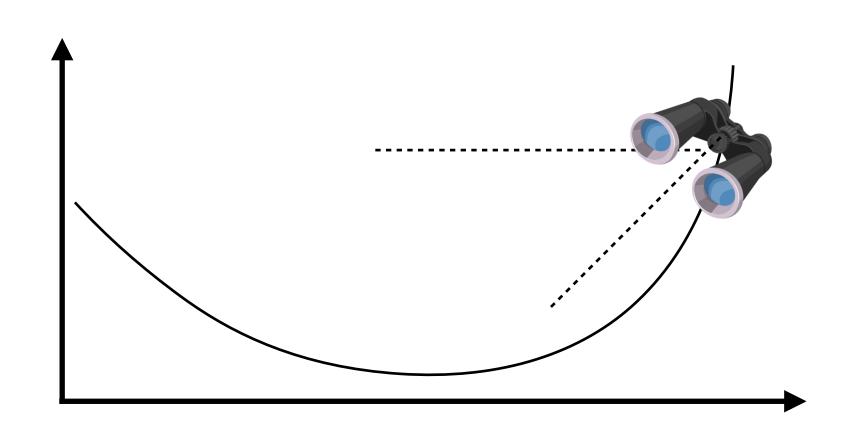
Find a solution whose value is not too far from the minimum

$$\forall x, f(\tilde{x}) \leq f(x^*) + \epsilon$$



# Terminology

#### Convex function

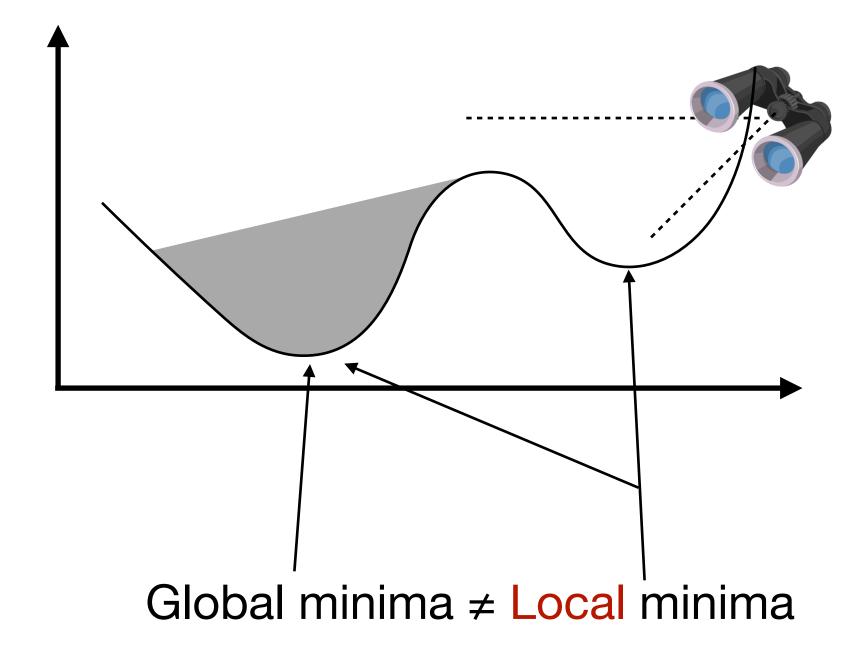


The entire graph is "visible" from any point

$$\forall t \in (0,1), f(tx + (1-t)y) \le tf(x) + (1-t)f(y)$$

Global minima = Local minima

#### Non-convex function



(in the context of continuous optimization)

# Great goal of quantum optimizers:

Find relevant optimization problems that can be solved much faster than with any classical algorithm

#### We are not there yet:

- Quantum optimization often lacks theoretical guarantees, or makes contrived assumptions
- Quantum advantages vanish under implementation overhead (ex: quantum error correction)
- New classical optimization methods fight back (ex: deep learning)

... but the field is emerging and first-gen quantum computers accelerate its development

### Quantum optimization algorithms

# Lecture 1 (Physics-inspired)

# Lecture 2 (Oracle-based)

#### Exact algorithms

- Quantum Phase Estimation (QPE)
- Quantum Adiabatic Algorithm (QAA)

#### Variational quantum algorithms

- Variational Quantum Eigensolver (VQE)
- Quantum Approximate Optimization
   Algorithm (QAOA)

#### Grover-type algorithms

- Quantum Minimum Finding
- Minimum Spanning Tree

#### Gradient computation

#### Monte-Carlo algorithms

- Linear programming
- Escaping Saddle Points

# Optimization as a physics problem

Linear operator encoding the possible energy levels of a system

$$H \in \mathbb{C}^{2^n \times 2^n}$$

Hermitian  $H^{\dagger} = H$ 

Eigendecomposition: 
$$H = \sum_{i=1}^{2^n} \lambda_i | v_i \rangle$$

Energy levels: real eigenval.  $\lambda_1 \leq \lambda_2 \leq \dots$ 

Stationary states: eigenvec.  $H|v_i\rangle = \lambda_i |v_i\rangle$ 

Smallest eigenvalue  $\lambda_1$  (lowest energy) and corresponding eigenvector  $|v_1\rangle$  (ground state) characterize the most stable configuration of the system

Linear operator encoding the possible energy levels of a system

$$H \in \mathbb{C}^{2^n \times 2^n}$$

Hermitian  $H^{\dagger} = H$ 

Example: A qubit in a magnetic field of angular frequency  $\omega$ 

$$H = \begin{pmatrix} \frac{\hbar\omega}{2} & 0 \\ 0 & -\frac{\hbar\omega}{2} \end{pmatrix}$$
 Eigenvectors:  $|0\rangle$  and  $|1\rangle$  (ground state) 
$$\frac{\hbar\omega}{2} - \frac{\hbar\omega}{2}$$
 (energies)

ħ: Dirac constant

Ground state computation is an optimization problem:

$$\lambda_1 = \|H\|v_1\rangle\| = \min_{|v\rangle \in \mathbb{C}^{2^n}: \|v\| = 1} \|H\|v\rangle\|$$
 optimized element ~  $x$ 

objective function  $\sim f(x)$ 

How hard is it to optimize?

- Diagonalization is infeasible in general (matrix of exponential size)
- Optimization landscape is highly complicated (non-convex)
- ... requires making additional assumptions on H (examples: next slide)

# Examples of more friendly Hamiltonians

#### Representation

$$H = \sum_{j=1}^{m} H_j$$

$$H = \begin{pmatrix} H_{11} H_{12} & \cdots & H_{12^n} \\ H_{21} & & \vdots \\ \vdots & & & \\ H_{2^{n_1}} & \cdots & H_{2^{n_2n}} \end{pmatrix}$$
Each row has at most  $k$  non-zero entries

#### k-local

Each  $H_j$  acts nontrivially only on k qubits

non-zero entries

#### Commuting

 $H_1, ..., H_m$  commute

#### Stoquastic

Off-diagonal terms are real and non-positive

#### Frustration-free

Ground state of H is also a ground state of  $H_1, \ldots, H_m$ 

Easy to optimize classically! arXiv:0806.1746

#### Non-degenerate $H = \sum \lambda_i | v_i \rangle$

Unique smallest eigenvalue  $\lambda_1 < \lambda_2$ 

Large gap between first two eigenvalues  $\lambda_2 - \lambda_1 > \Delta$ 

#### Structural properties of ground state

Complexity, area laws, ...

Ground state computation is an optimization problem:

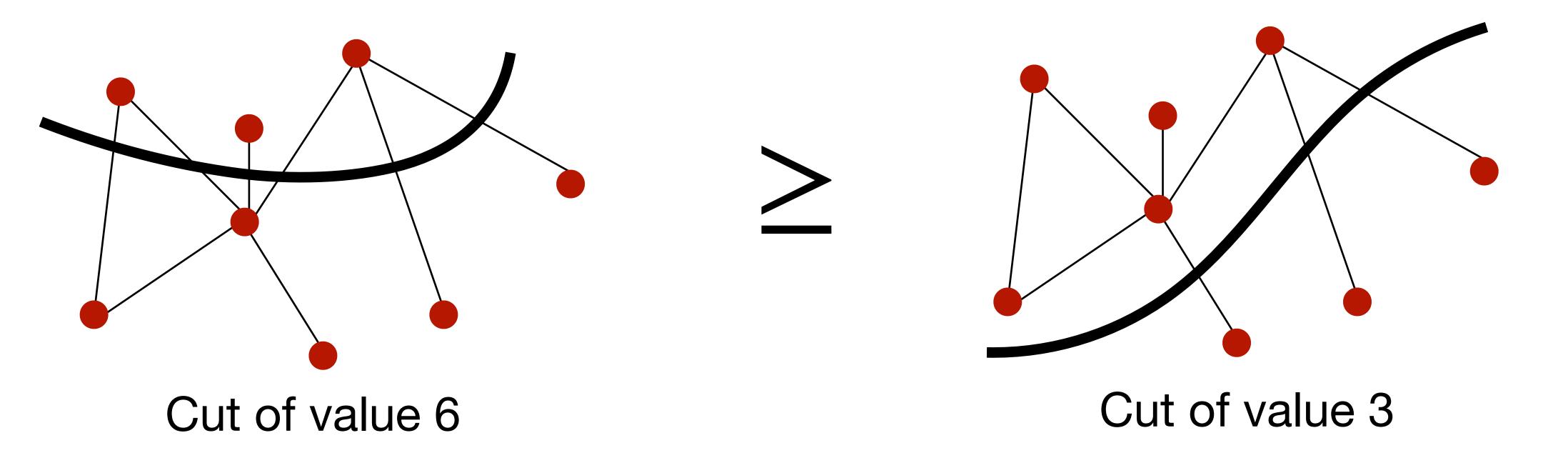
$$\lambda_1 = ||H||v_1\rangle|| = \min_{|v\rangle \in \mathbb{C}^{2^n}: ||v|| = 1} ||H||v\rangle||$$

#### How useful/general is it?

- Ground state reveals physical properties (electronic configurations, phases
  of matter...) exploited in quantum chemistry, condensed matter physics, etc.
- Lots of other optimization problems can be reduced to it
   Example (next slide): combinatorial optimization via QUBO Hamiltonian

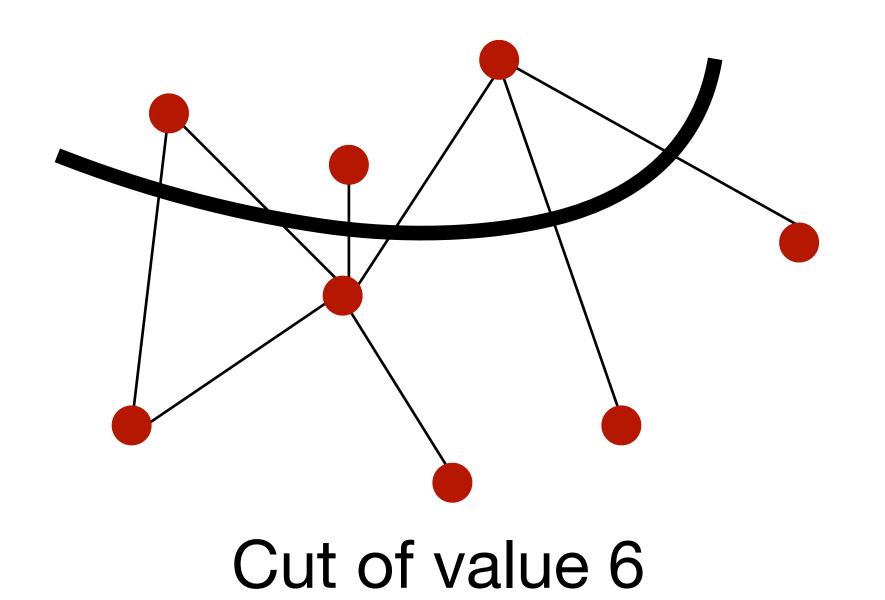
#### Max-Cut problem

Partition vertices of a graph into two parts that maximize number of edges between the two



#### Max-Cut problem

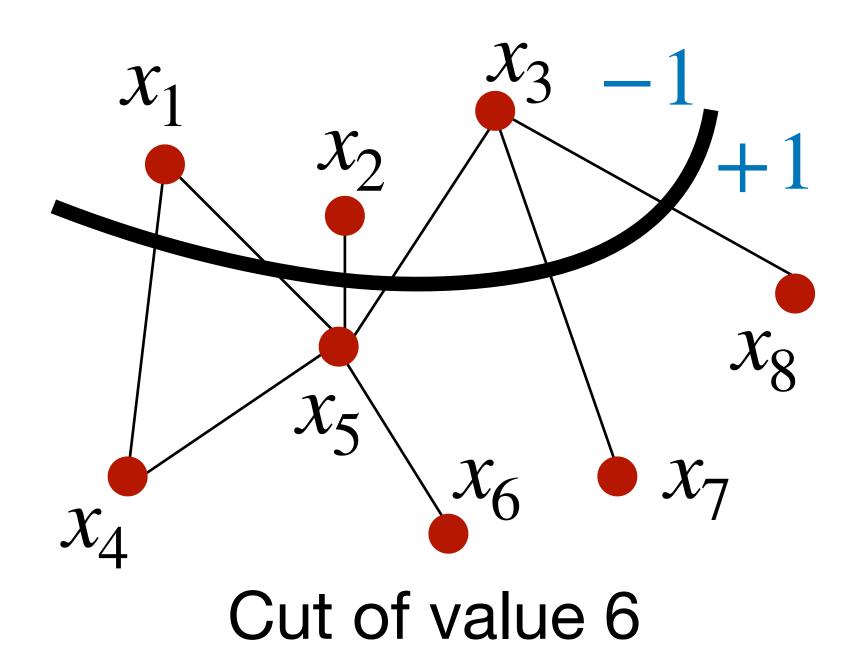
Partition vertices of a graph into two parts that maximize number of edges between the two



- Fundamental problem in discrete optimization
- NP-Hard
- Famous classical approximation algo.
   (Goemans-Williamson)

#### Max-Cut problem

Partition vertices of a graph into two parts that maximize number of edges between the two



How to encode it into a Hamiltonian?

Max-Cut = 
$$\min_{x \in \{-1,1\}^n} \sum_{\{i,j\} \in \text{Edge}} -\frac{1}{4} (x_i - x_j)^2 f(x)$$

= ground state of

$$H = \begin{pmatrix} x \\ --f(x) \\ 0 \end{pmatrix} = \sum_{\{i,j\} \in \text{Edge}} \frac{1}{4} (Z_i - Z_j)^2$$

What other polynomials can be converted into Ising Hamiltonians?

QUBO (Quadratic unconstrained binary optimization)

$$\min_{x \in \{0,1\}^n} x^{\mathsf{T}} Q x = \min_{x \in \{0,1\}^n} \sum_{i,j} Q_{i,j} x_i x_j \qquad Q \in \mathbb{R}^{n \times n} \text{ symmetric}$$

Exercise: show that substituting  $x_i \mapsto (\mathrm{Id} - Z_i)/2$  yields a Hermitian matrix

# QUBO encompasses a lot of optimization problems



**Condensed Matter > Statistical Mechanics** 

[Submitted on 23 Feb 2013 (v1), last revised 24 Jan 2014 (this version, v3)]

#### Ising formulations of many NP problems

#### **Andrew Lucas**

We provide Ising formulations for many NP-complete and NP-hard problems, including all of Karp's 21 NP-complete problems. This collects and extends mappings to the Ising model from partitioning, covering and satisfiability. In each case, the required number of spins is at most cubic in the size of the problem. This work may be useful in designing adiabatic quantum optimization algorithms.

# ... but no guarantee in general that "QUBO" Hamiltonian is nice:

- small spectral gap
- long-range interactions
- lots an ancillae (higher dim.)
- ...

Ground state computation is an optimization problem:

$$\lambda_1 = ||H||v_1\rangle|| = \min_{|v\rangle \in \mathbb{C}^{2^n}: ||v|| = 1} ||H||v\rangle||$$

#### Why quantum computers may be useful here?

- They can solve the Schrödinger equation at a much lower cost  $Sim_H$  than classical algorithms (for "friendly" H)

$$i\frac{d|\psi(t)\rangle}{dt} = H|\psi(t)\rangle \xrightarrow{\text{Ham. simulation}} |\psi(1)\rangle = e^{-iH}|\psi(0)\rangle$$

- ... not clear yet how simulation relates to optimization Example (next parts): Quantum Phase Estimation, Adiabatic algorithm

# Exact Algorithms

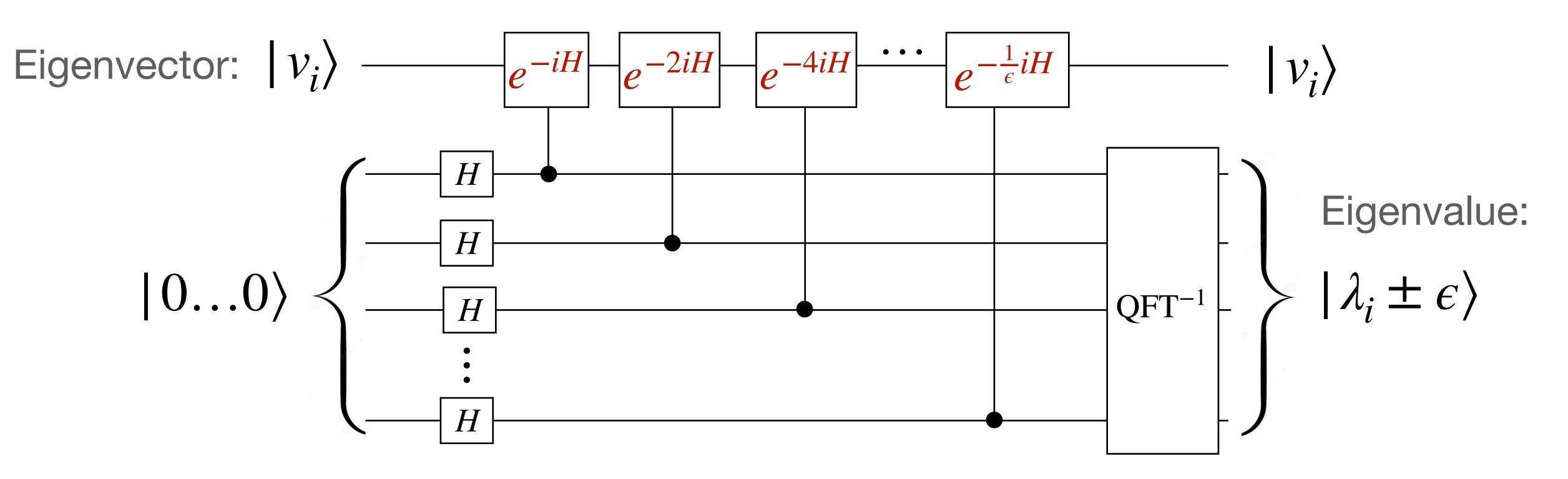
Quantum optimization algorithms that provably return the exact ground state

# Quantum Phase Estimation

#### Phase estimation circuit

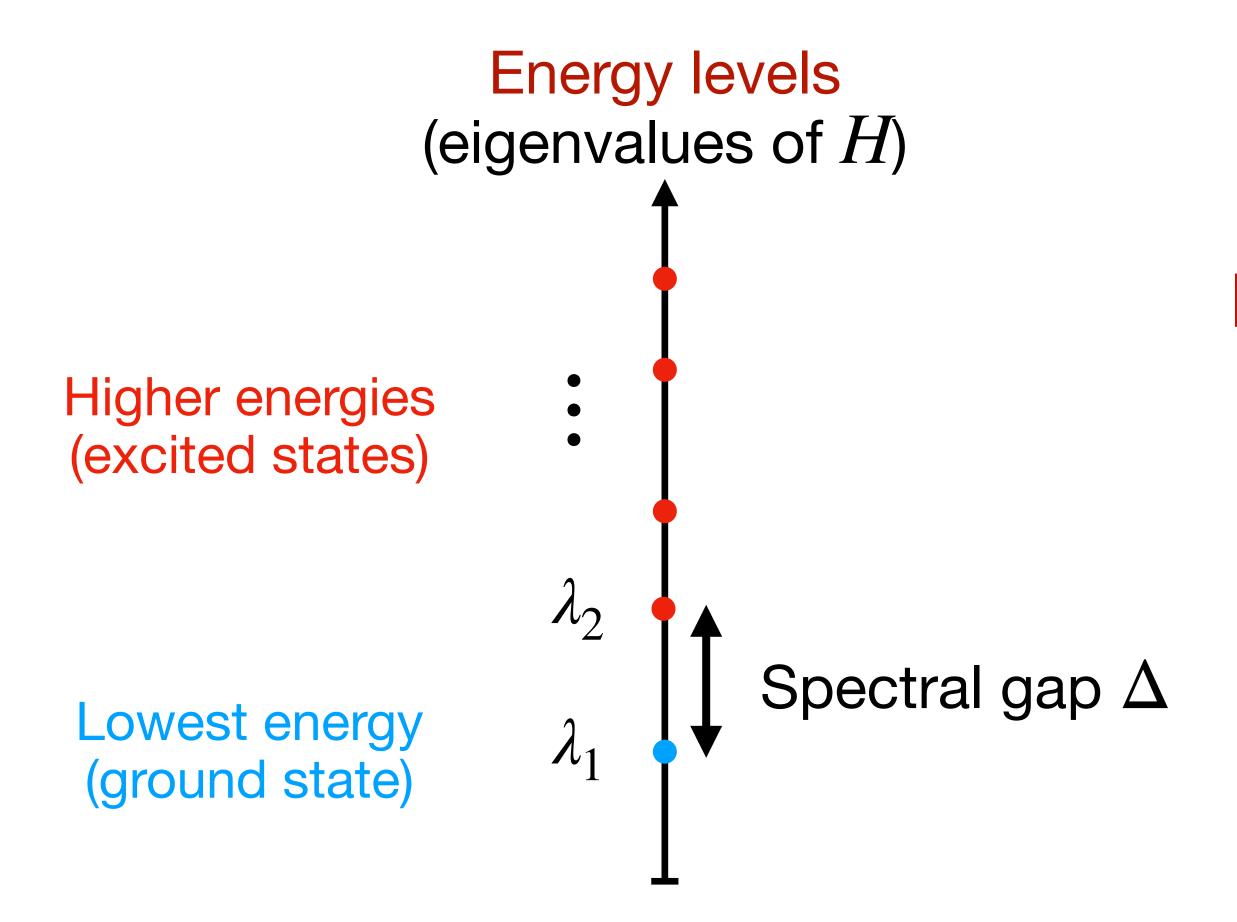
#### Allows computing energy levels of H

#### Hamiltonian simulation



Cost: 
$$\sim \epsilon^{-1} \times \text{Sim}_H$$

#### Precision needed by Phase estimation



Estimating the eigenvalues with precision  $\epsilon < \Delta$  allows distinguishing ground state from excited states

**Problem:** eigenstates are not known a priori, what input should be provided to Phase estimation?

#### Warm-starts

= states with best-possible overlap with ground state

# General purpose quantum optimizer

Warm-start (decomposition into eigenbasis of H)

Quantum Phase Estimation

Amplitude amplification

$$|\psi(0)\rangle = \sum_{i} \alpha_{i} |v_{i}\rangle \longrightarrow \sum_{i} \alpha_{i} |v_{i}\rangle |\lambda_{i} \pm \Delta\rangle \longrightarrow |v_{1}\rangle |\lambda_{1} \pm \Delta\rangle$$

Cost: 
$$|\langle \psi(0) | v_1 \rangle|^{-1} \times \sim \Delta^{-1} \times \text{Sim}_H$$

- Can provide the exact ground state
- Few assumptions required (H gapped and efficiently simulatable)
- Requires complicated quantum circuits (long coherence time, error correction...)
- Requires very good warm start (large overlap  $\langle \psi(0) | v_1 \rangle$ )

  Next part: relax this requirement

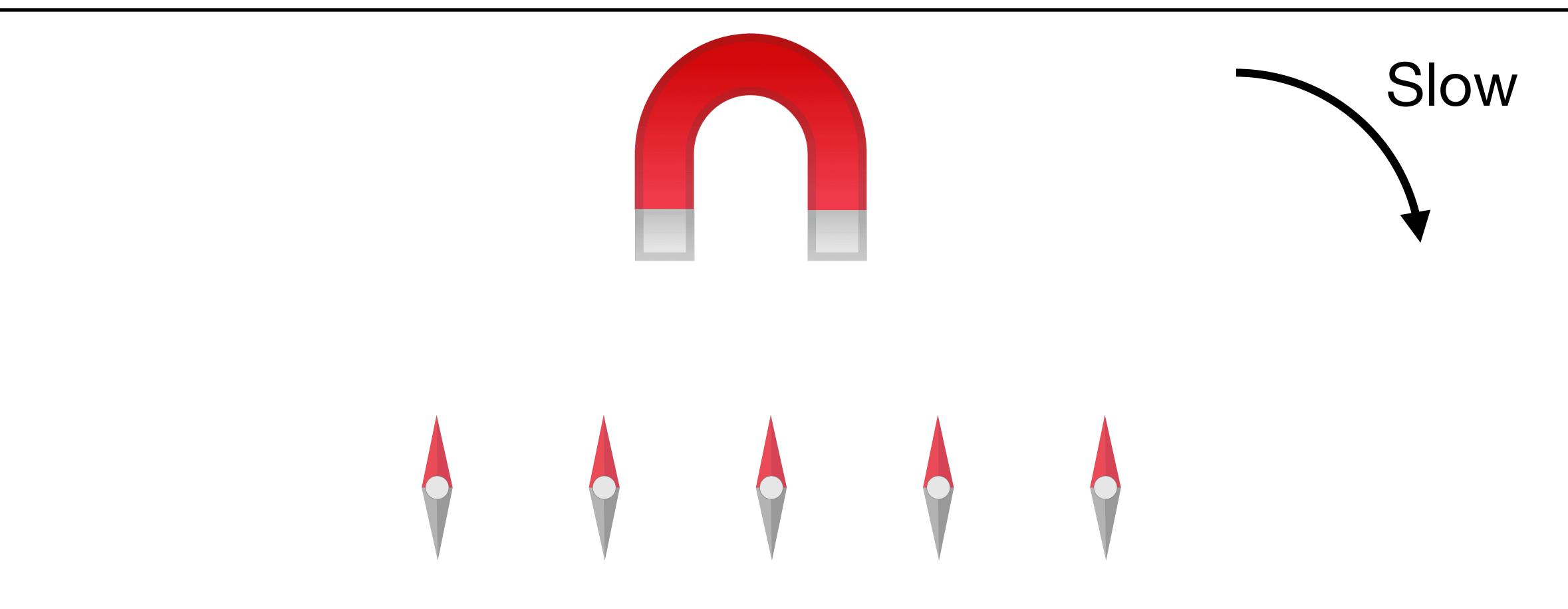
# Quantum Adiabatic Algorithm

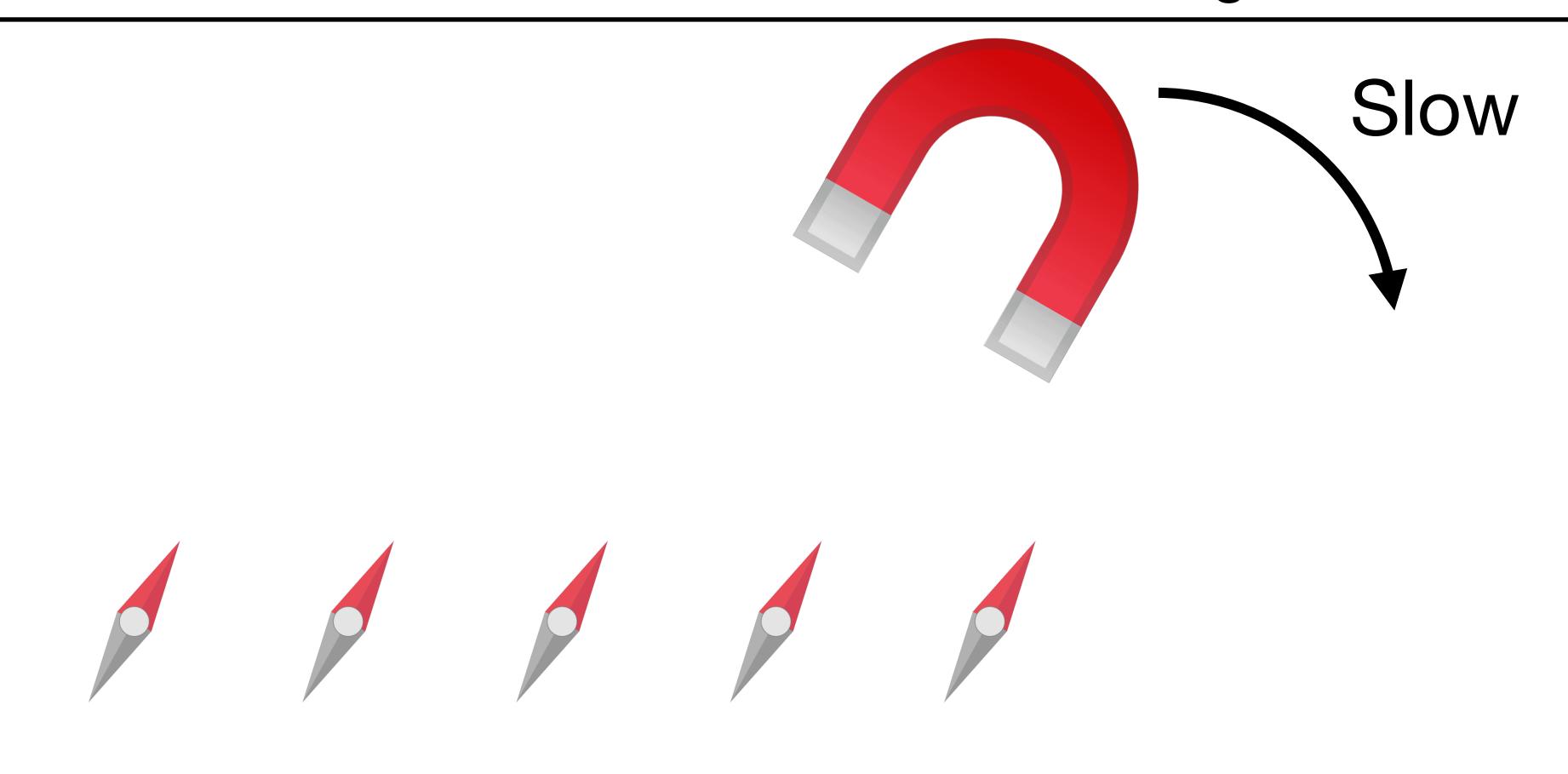
# Bootstrapping an approximate ground state

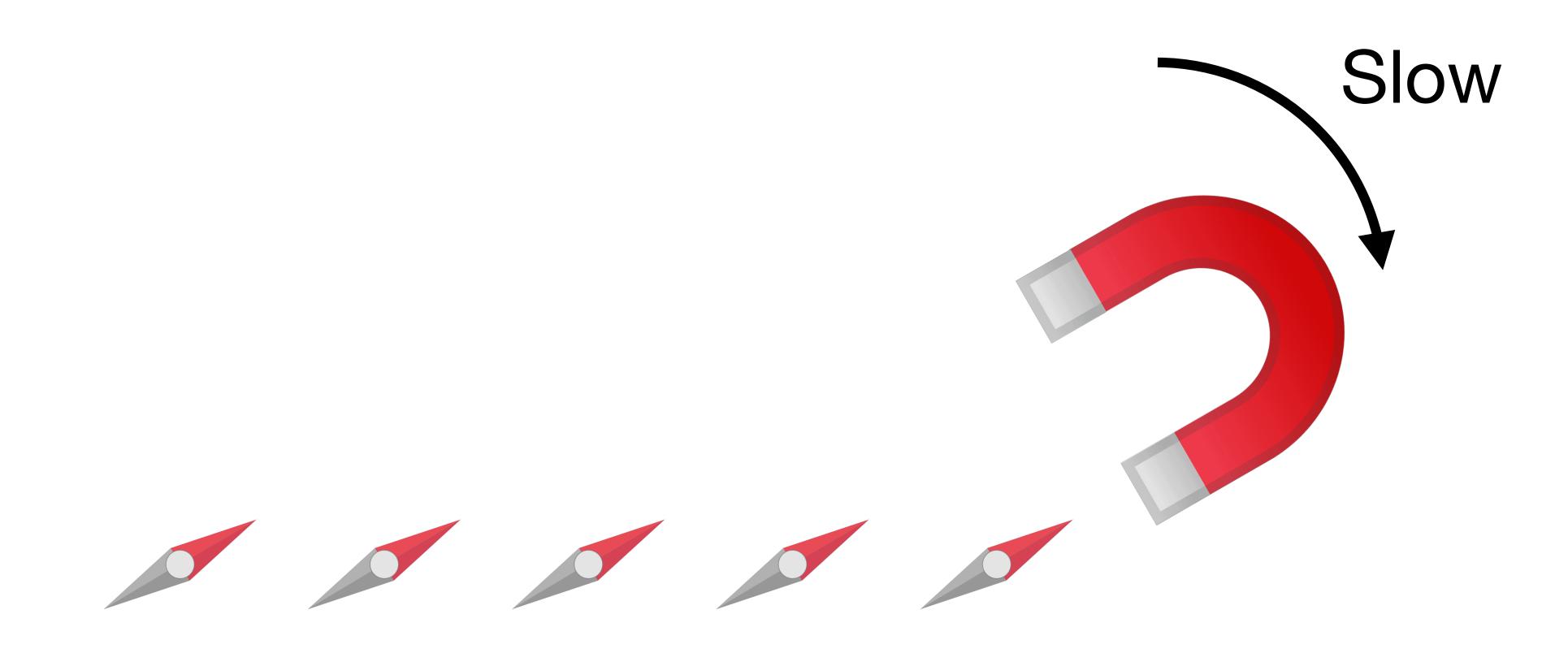
If we slightly perturb a Hamiltonian, its ground state should remain approximately the same.

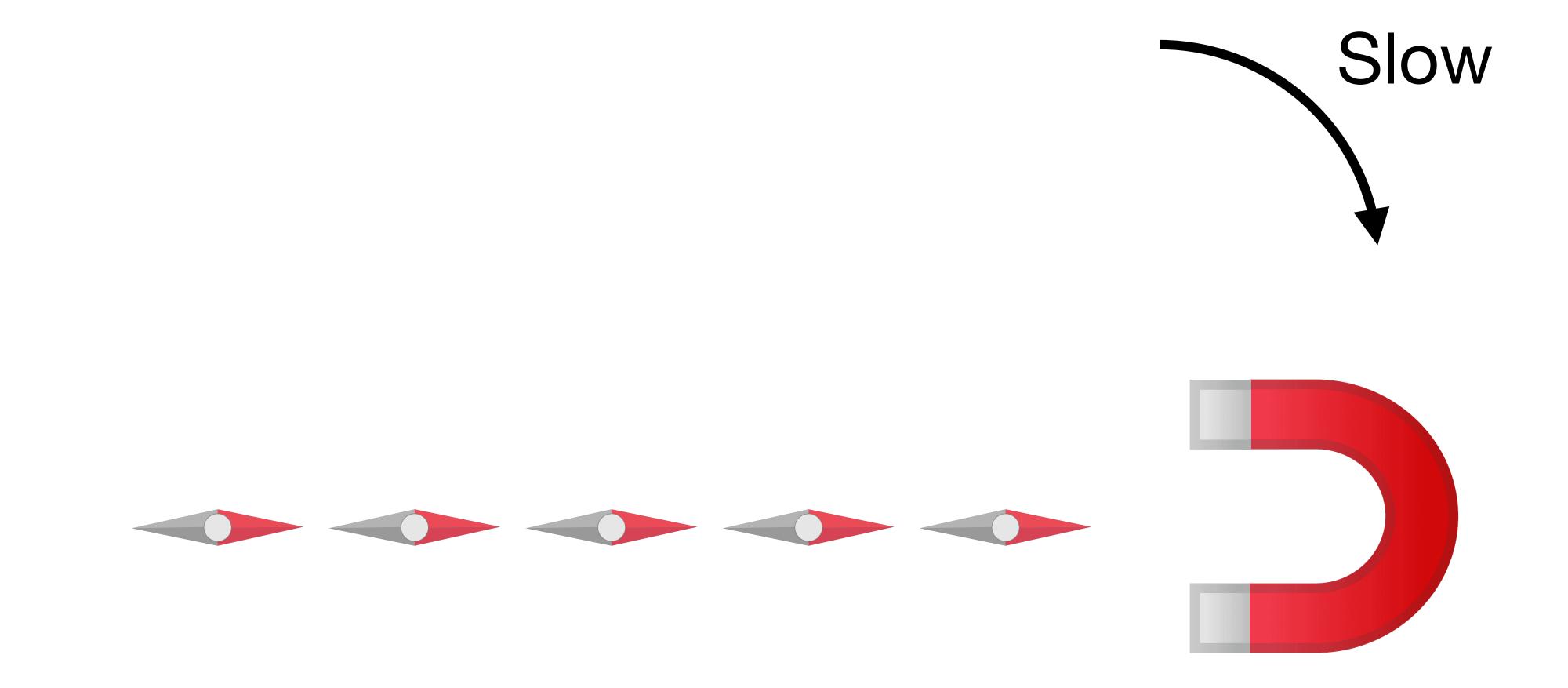
- Large overlap  $|\langle v_1 | w_1 \rangle|$
- Use  $|v_1\rangle$  as a warm-start to prepare  $|w_1\rangle$

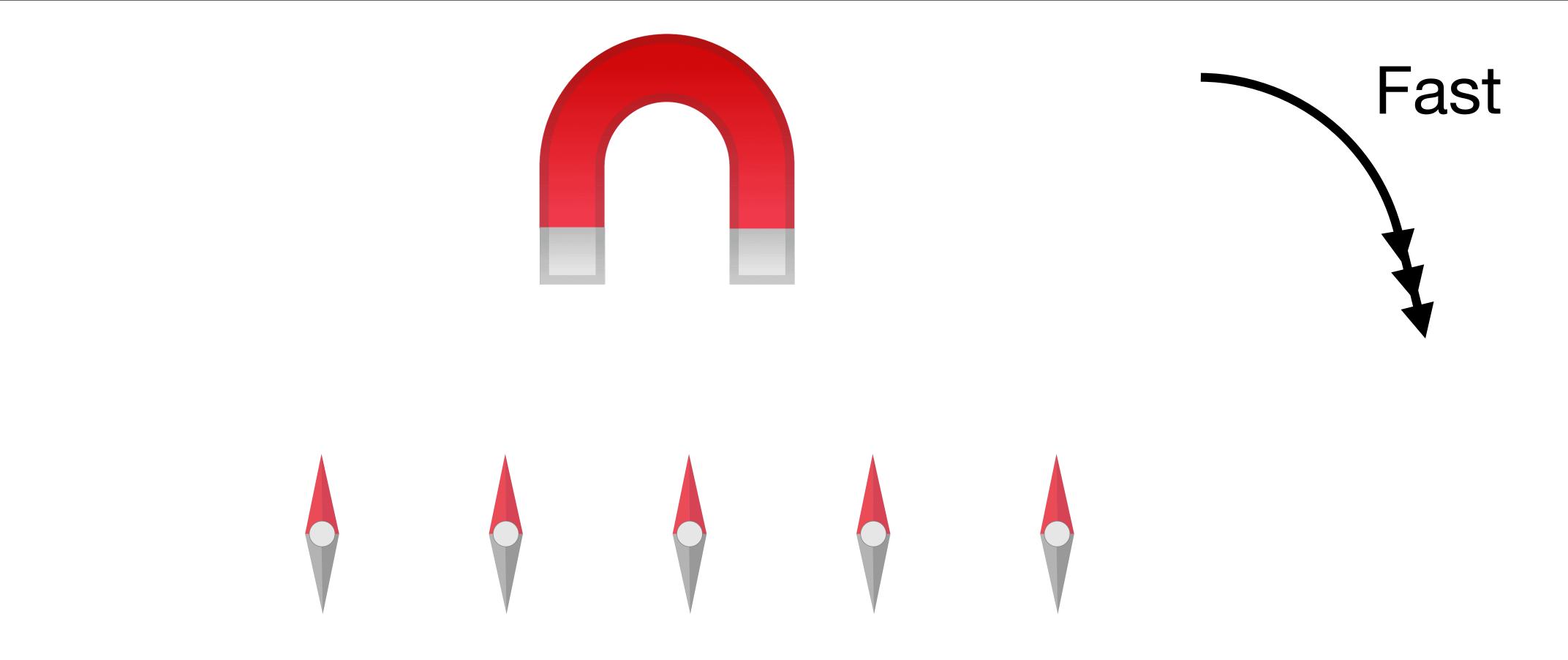
- Large overlap  $|\langle w_1 | u_1 \rangle|$
- Use  $|w_1\rangle$  as a warm-start to prepare  $|u_1\rangle$

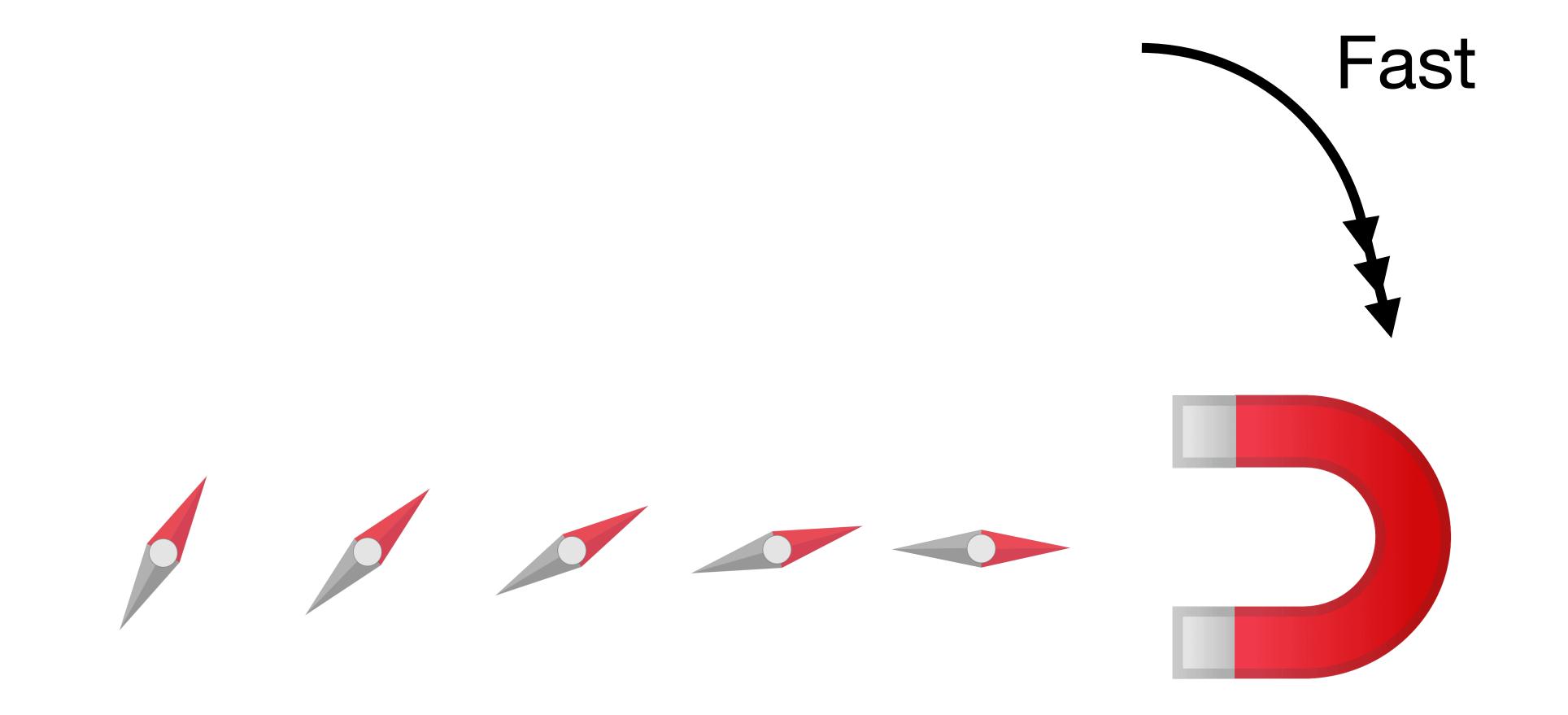












If a system is initialized in the ground state of a Hamiltonian H(t) that evolves slowly over time, then it remains in the instantaneous ground state.

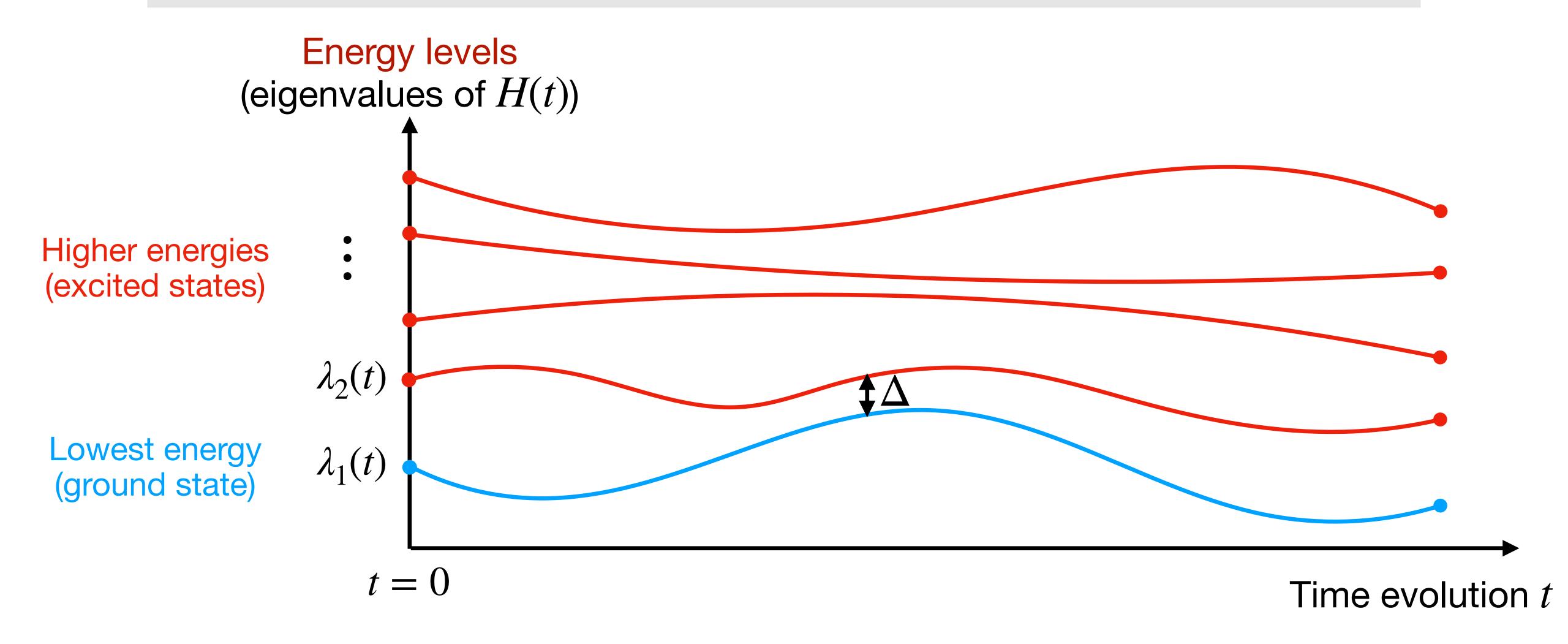
$$i\frac{d|\psi(t)\rangle}{dt} = H(vt)|\psi(t)\rangle$$

evolution slowed-down at speed  $v \in (0,1]$ 

#### Time-dependent Hamiltonians:

- Eigenvalues and eigenvectors can also evolve over time
- Schrödinger equation has no analytical solution in general

# Energy spectrum of time-evolving Hamiltonian



Assumption: no level crossings (nonzero energy gap  $\Delta$  between ground and excited states throughout the evolution)

# Adiabatic Theorem (simplified)

If a system is initialized in the ground state of a Hamiltonian H(t) that evolves slowly over time, then it remains in the instantaneous ground state.

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

evolution slowed-down at speed  $v \in (0,1]$ 

Minimum spectral gap: 
$$\Delta = \min_{0 \le t \le 1} \lambda_2(t) - \lambda_1(t)$$
 Cost:  $\sim 1/\nu \times Sim_H$ 

If  $|\psi(0)\rangle$  is the ground state of H(0) and  $v \lesssim \Delta^2 \cdot \epsilon \cdot (\|\dot{H}(0)\| + \|\dot{H}(1)\| + \max_t \|\ddot{H}(t)\|^2 + \|\dot{H}(t)\|^3/\Delta)^{-1}$  then the solution  $|\psi(1)\rangle$  to the Schrödinger eq. at t=1 is  $\epsilon$ -close to the ground state of H(1)

# Applying the Adiabatic Theorem

 $H_1$ : target Hamiltonian whose ground state is sought (ex: QUBO Hamiltonian)

$$H_1 = -\sum_{i,i} (Z_i - Z_j)^2$$

 $H_0$ : starting Hamiltonian whose ground state is easy to prepare (ex: transverse field Hamiltonian)

$$H_0 = -\sum_i X_i$$

H(t): interpolating Hamiltonian with  $H(0) = H_0$  and  $H(1) = H_1$  (ex: line interpolation)

$$H(t) = (1 - t)H_0 + tH_1$$

#### Requirements:

- $H_0$  and  $H_1$  do not commute (or it leads to level crossings)
- Spectral gap  $\Delta$  is large (allows fast evolution speed  $\nu$ )
- H(t) can be simulated efficiently (depends on hardware restrictions)

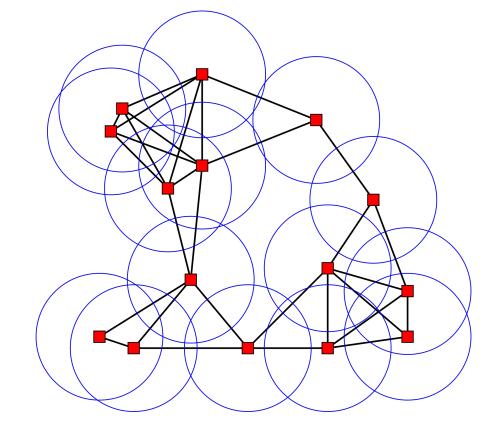
# Applying the Adiabatic Theorem

Caveat 1: spectral gap  $\Delta$  is often exponentially small or unknown

Caveat 2: choice of Hamiltonian is constrained by type of analog quantum computer

#### Example:

Rydberg atom arrays (as used by Pasqal or QuEra) implement interactions corresponding to unit disk graphs



Adiabatic algorithm can also be run on digital, circuit-based computers (discretized adiabatic evolution, randomized evolutions, ...)

Caveat 3: requires sustained coherence throughout the entire runtime

#### (Sub)Exponential advantage of adiabatic Quantum computation with no sign problem



András Gilyén,



Matthew B. Hastings,



Umesh Vazirani

Authors Info & Claims

STOC 2021: Proceedings of the 53rd Annual ACM SIGACT Symposium on Theory of Computing Pages 1357 - 1369 • https://doi.org/10.1145/3406325.3451060

Published: 15 June 2021 Publication History



#### Abstract

We demonstrate the possibility of (sub)exponential quantum speedup via a quantum algorithm that follows an adiabatic path of a gapped Hamiltonian with no sign problem. The Hamiltonian that exhibits this speed-up comes from the adjacency matrix of an undirected graph whose vertices are labeled by *n*-bit strings, and we can view the adiabatic evolution as an efficient O(poly(n))-time quantum algorithm for finding a specific "EXIT" vertex in the graph given the "ENTRANCE" vertex. On the other hand we show that if the graph is given via an adjacency-list oracle, there is no classical algorithm that finds the "EXIT" with probability greater than  $\exp(-n^{\delta})$  using at most  $\exp(n^{\delta})$  queries for  $\delta = 1/5 - o(1)$ . Our construction of the graph is somewhat similar to the "welded-trees" construction of Childs et al., but uses additional ideas of Hastings for achieving a spectral gap and a short adiabatic path.

There are Hamiltonians with properties similar to those in QUBO optimization (stoquastic), for which the adiabatic algorithm is provably much faster than any classical optimization algorithm

... but these Hamiltonians are somewhat artificial

# Variational quantum algorithms

Reduce the search space to a smaller region than can be efficiently explored using a combination of classical + quantum computing

# Variational Quantum Eigensolver (VQE)

# The variational method

Ground state computation is an optimization problem:

$$\lambda_1 = ||H||v_1\rangle|| = \min_{|v\rangle \in \mathbb{C}^{2^n}: ||v|| = 1} ||H||v\rangle||$$

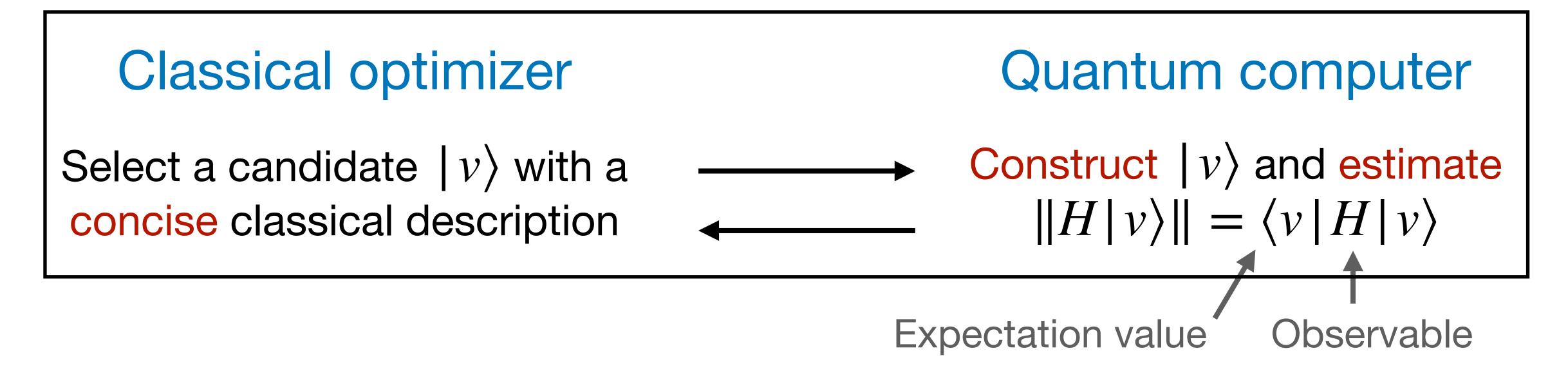
#### What if we use classical optimization solvers?

- Elements from the search space  $|v\rangle \in \mathbb{C}^{2^n}$  can be difficult to store and manipulate on classical computers (exponential dimension)
- Objective function  $||H|v\rangle||$  can be hard to evaluate

Variational method: hybrid quantum-classical optimizers

# The variational method

The evaluation of the objective function is delegated to a quantum computer



The classical optimizer refines its solution by making iterative calls to a quantum computer

# The variational method

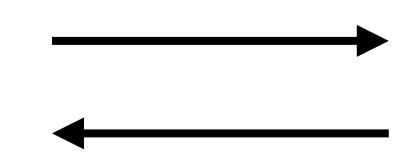
- Requires fewer quantum resources than full-fledged quantum algorithms
- A leading proposal for near-term quantum applications
- Tested in practice (ex: hybrid computing platform being installed at the French supercomputing center TGCC)
- Highly heuristic... but so is classical optimization on such problems

# Variational Quantum Eigensolver

#### Classical optimizer

Quantum computer

Select a candidate  $|v\rangle$  with a concise classical description



Construct 
$$|v\rangle$$
 and estimate  $|H|v\rangle| = \langle v|H|v\rangle$ 

#### How to represent the candidate states?

Classical parameters  $(N \ll 2^n)$ 

Quantum state

Ansatz:

$$(\theta_1, \ldots, \theta_N)$$

 $|v(\theta_1,...,\theta_N)\rangle$ 

Example (next part): the QAOA ansatz

# Energy estimation

#### Classical optimizer

#### Quantum computer

Select parameters 
$$(\theta_1, ..., \theta_N)$$

Construct  $|v(\theta_1,...,\theta_N)\rangle$  and estimate  $|H|v(\theta_1,...,\theta_N)\rangle|$ 

The energy estimation  $|H|v\rangle|$  could be performed using Quantum Phase Estimation, but this would make the algorithm incompatible with near-term quantum architectures.

Instead, we typically rely on random measurement strategies based on prior knowledge about H (ex: if H is a QUBO Hamiltonian, we can average multiple measurements in the standard basis)

### Barren Plateaus

The choice of the variational ansatz is crucial in making the method succeed

Highly expressive ansätze (i.e., those spanning a large region of the original search space) are more likely to cause the classical optimizer to get stuck in local minima

#### Phenomenon known as Barren Plateaus:

For a given observable H over n qubits, all but an exponentially small fraction of the quantum states  $|v\rangle \in \mathbb{C}^{2^n}$  have energy exponentially close to the average:  $|H|v\rangle |= \mathrm{Tr}(H)/2^n \pm 2^{-\Omega(n)}$ . (i.e., the optimization landscape is nearly flat over a large sub-region)

# Quantum Approximate Optimization Algorithm (QAOA)

QAOA instantiates the Variational Quantum Eigensolver with an ansatz inspired by the Quantum Adiabatic Algorithm.

# Trotterized adiabatic evolution

Recall: The adiabatic algorithm solves the Schrödinger equation  $i\frac{d|\psi(t)\rangle}{dt}=H(t)|\psi(t)\rangle.$ 

Goal: Understand what the ground state  $|\psi(1)\rangle$  looks like to derive an ansatz

Continuous-time Hamiltonian H(t) can be approximated by a finite sequence:

 $H(0), H(\delta), H(2\delta), \dots, H(1)$  for a sufficiently small time step  $\delta \ll 1$ .

By solving the corresponding sequence of Schrödinger equations,

$$|\psi(1)\rangle_{\stackrel{\delta}{\delta} \to 0} = e^{-i\delta H(1)}...e^{-i\delta H(2\delta)}e^{-i\delta H(\delta)}e^{-i\delta H(0)}|\psi(0)\rangle$$

# Trotterized adiabatic evolution

$$|\psi(1)\rangle = e^{-i\delta H(1)}...e^{-i\delta H(2\delta)}e^{-i\delta H(\delta)}e^{-i\delta H(0)}|\psi(0)\rangle$$

Suppose H(t) is given by the line interpolation  $H(t) = (1 - t) H_0 + t H_1$ 

Each unitary can be expanded as follows:

$$e^{-i\delta H(j\delta)} = e^{-i\delta(1-j\delta)} \frac{H_0 - ij\delta^2 H_1}{H_0} \neq e^{-i\delta(1-j\delta)} \frac{H_0 - ij\delta^2 H_1}{H_0} = e^{-i\delta(1-j\delta)} \frac{H_0 - ij\delta^2$$

### Trotterized adiabatic evolution

Putting everything together:

$$|\psi(1)\rangle = \prod_{\substack{\delta \to 0 \\ \delta' \to 0}} \frac{1/\delta}{i=0} \left( e^{-i\delta'\delta(1-j\delta)H_0} e^{-ij\delta'\delta^2 H_1} \right)^{1/\delta'} |\psi(0)\rangle$$

Ground state is obtained by alternating small evolutions according to  $H_0$  or  $H_1$ 

For any  $\epsilon \in (0,1)$ , there exists a depth p and a sequence of angles  $\theta_1,\theta_2,\ldots,\theta_{2p} \in [0,2\pi]$  such that,

$$|\psi(1)\rangle \approx_{\epsilon} e^{-i\theta_{2p}H_{0}}e^{-i\theta_{2p-1}H_{1}}\cdots e^{-i\theta_{3}H_{1}}e^{-i\theta_{2}H_{0}}e^{-i\theta_{1}H_{1}}|\psi(0)\rangle$$

# The QAOA ansatz

QAOA explores ansätze of the form:

$$|v(\theta_1,...,\theta_p)\rangle = e^{-i\theta_{2p}H_0}e^{-i\theta_{2p-1}H_1}...e^{-i\theta_3H_1}e^{-i\theta_2H_0}e^{-i\theta_1H_1}|\psi(0)\rangle$$

where, typically, p is much smaller than what is required by Trotter approximation.

Advantage over adiabatic algorithm: low-depth quantum circuits

Search space with p = 1 already encompass some interesting states:

Non-trivial approximate solutions to QUBO Hamiltonians (ex: Max-Cut on 3-regular graphs)

Measurement distributions that cannot be efficiently classically sampled from

Significant speedups for certain Constraint Satisfaction Problems over best-known classical algorithms

arXiv:1411.4028 arXiv:1602.07674 arXiv:2411.04979

... but provable speedups remain elusive and QAOA ansatz is harder to analyse for p>1

# Quantum optimization algorithms

# Lecture 1 (Physics-inspired)

# Lecture 2 (Oracle-based)

#### Exact algorithms

- Quantum Phase Estimation (QPE)
- Quantum Adiabatic Algorithm (QAA)

#### Variational quantum algorithms

- Variational Quantum Eigensolver (VQE)
- Quantum Approximate Optimization
   Algorithm (QAOA)

#### Grover-type algorithms

- Quantum Minimum Finding
- Minimum Spanning Tree

#### Gradient computation

#### Monte-Carlo algorithms

- Linear programming
- Escaping Saddle Points