Week 11: Hamiltonians and Quantum Simulation

COMS 4281 (Fall 2024)

Admin

1. Worksheet and Quiz 6 out tonight.
2. Pset2 will be out this weekend, and due December 4.
3. Final in-class exam on December 9.

Hamiltonians

In quantum physics, **Hamiltonians** describe the laws of nature of a quantum system. In principle, they encode all information about how a collection of particles (in isolation) interact with each other over time.

Hamiltonians

In quantum physics, **Hamiltonians** describe the laws of nature of a quantum system. In principle, they encode all information about how a collection of particles (in isolation) interact with each other over time.

Arguably, the **killer app** of quantum computing is **Hamiltonian simulation**, which is to evolve a quantum state over a time according to a Hamiltonian.

Linear algebra review

Spectral theorem

Let $A \in \mathbb{C}^{d \times d}$ be a Hermitian matrix. It can always be **diagonalized**.

Spectral theorem

Let $A \in \mathbb{C}^{d \times d}$ be a Hermitian matrix. It can always be **diagonalized**.

There exists an **orthonormal basis** $\{|v_1\rangle, \ldots, |v_d\rangle\}$ for $\mathbb{C}^d$ and **real eigenvalues** $\lambda_1, \ldots, \lambda_d$ such that

$$A = \sum_{j=1}^{d} \lambda_j |v_j\rangle\langle v_j|$$

Spectral theorem

Let $A \in \mathbb{C}^{d \times d}$ be a Hermitian matrix. It can always be **diagonalized**.

There exists an **orthonormal basis** $\{|v_1\rangle, \ldots, |v_d\rangle\}$ for $\mathbb{C}^d$ and **real eigenvalues** $\lambda_1, \ldots, \lambda_d$ such that

$$A = \sum_{j=1}^{d} \lambda_j |v_j\rangle\langle v_j|$$

This is called a **spectral decomposition** of A.

Spectral theorem

In other words, A looks like

$$A = V \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_d \end{pmatrix} V^\dagger$$

where V is a **unitary matrix** with $|v_j\rangle$ as its columns.

Spectral theorem

The vector $|v_k\rangle$ has eigenvalue λ_k with respect to A.

Spectral theorem

The vector $|v_k\rangle$ has eigenvalue λ_k with respect to A.

Proof: $A|v_k\rangle = \left(\sum_j \lambda_j |v_j\rangle\langle v_j|\right)|v_j\rangle$

Spectral theorem

The vector $|v_k\rangle$ has eigenvalue λ_k with respect to A.

Proof: $A|v_k\rangle = \left(\sum_j \lambda_j |v_j\rangle\langle v_j|\right)|v_j\rangle$

$= \sum_j \lambda_j |v_j\rangle \langle v_j \mid v_k\rangle$

Spectral theorem

The vector $|v_k\rangle$ has eigenvalue λ_k with respect to A.

Proof: $A|v_k\rangle = \left(\sum_j \lambda_j |v_j\rangle\langle v_j|\right)|v_j\rangle$

$= \sum_j \lambda_j |v_j\rangle \langle v_j \mid v_k\rangle$

$= \lambda_k |v_k\rangle$ because $\langle v_j \mid v_k\rangle = 1$ only when $j = k$.

Functions of Hermitian matrices

Let $f : \mathbb{R} \to \mathbb{C}$ denote a function. Then for all Hermitian matrices A with spectral decomposition $\sum_j \lambda_j |v_j\rangle\langle v_j|$, we define

$$f(A) = \sum_j f(\lambda_j)\, |v_j\rangle\langle v_j|.$$

Functions of Hermitian matrices

Let $f : \mathbb{R} \to \mathbb{C}$ denote a function. Then for all Hermitian matrices A with spectral decomposition $\sum_j \lambda_j |v_j\rangle\langle v_j|$, we define

$$f(A) = \sum_j f(\lambda_j)\, |v_j\rangle\langle v_j|.$$

In other words, f just changes the **eigenvalues** of A, and leaves the eigenvectors unchanged.

Functions of Hermitian matrices

Example: let $f(x) = x^2$. Then

$f(A) = \sum_j \lambda_j^2 |v_j\rangle\langle v_j|$.

Functions of Hermitian matrices

Example: let $f(x) = x^2$. Then

$f(A) = \sum_j \lambda_j^2 |v_j\rangle\langle v_j|$.

This matches

$$A^2 = \Big(\sum_j \lambda_j |v_j\rangle\langle v_j|\Big)\Big(\sum_k \lambda_k |v_k\rangle\langle v_k|\Big)$$
$$= \sum_{j,k} \lambda_j \lambda_k \, |v_j\rangle \, \langle v_j \mid v_k\rangle \, \langle v_k|$$

Functions of Hermitian matrices

Example: let $f(x) = x^2$. Then

$f(A) = \sum_j \lambda_j^2 |v_j\rangle\langle v_j|$.

This matches

$$A^2 = \Big(\sum_j \lambda_j |v_j\rangle\langle v_j|\Big)\Big(\sum_k \lambda_k |v_k\rangle\langle v_k|\Big)$$
$$= \sum_{j,k} \lambda_j \lambda_k \, |v_j\rangle \, \langle v_j \mid v_k\rangle \, \langle v_k|$$
$$= \sum_j \lambda_j^2 |v_j\rangle\langle v_j|$$

Functions of Hermitian matrices

Example: let $f(x) = \sin(x)$. Then

$f(A) = \sum_j \sin(\lambda_j) \, |v_j\rangle\langle v_j|$.

The computer science perspective of Hamiltonians

If you take a physics class, you learn about Hamiltonians as the sum of potential and kinetic energy operators of a system, and their connection to equations of motion, etc., etc., etc...

If you take a physics class, you learn about Hamiltonians as the sum of potential and kinetic energy operators of a system, and their connection to equations of motion, etc., etc., etc...

Before we dive into the physics, let's first see how computer scientists think about Hamiltonians.

If you take a physics class, you learn about Hamiltonians as the sum of potential and kinetic energy operators of a system, and their connection to equations of motion, etc., etc., etc...

Before we dive into the physics, let's first see how computer scientists think about Hamiltonians.

CS view of Hamiltonians: Hamiltonians are **quantum analogues** of constraint satisfaction problems (CSPs).

Constraint satisfaction problems

An instance of a k-**local CSP** consists of:

- **variables** $x_1, \ldots, x_n$ that can take boolean values
- **constraints** $C_1, \ldots, C_m$ where each C_j indicates the allowed values for a subset S_j of variables.

Constraint satisfaction problems

An instance of a k-**local CSP** consists of:

- **variables** $x_1, \ldots, x_n$ that can take boolean values
- **constraints** $C_1, \ldots, C_m$ where each C_j indicates the allowed values for a subset S_j of variables.

Example: **3SAT** is a 3-local CSP where each of the constraints C_j are of the form

$$C_j = x_1 \vee x_5 \vee \neg x_7$$

Constraint satisfaction problems

The important questions: given a CSP,

1. Is it **satisfiable**?
2. What is the maximum number of constraints that can be simultaneously satisfied?

Constraint satisfaction problems

The important questions: given a CSP,

1. Is it **satisfiable**?
2. What is the maximum number of constraints that can be simultaneously satisfied?

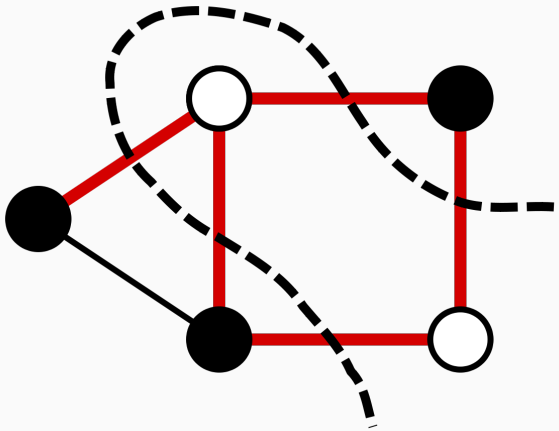
These questions generally correspond to **NP-complete problems**.

Max-Cut Problem

Given a graph $G = (V, E)$, find a partition of vertices that maximizes number of cut edges.

Max-Cut Problem

Given a graph $G = (V, E)$, find a partition of vertices that maximizes number of cut edges.



Equivalently, a 2-local CSP: - For every vertex $v \in V$, a variable x_v. - For every edge $e = (u, v) \in E$, a constraint $x_u \neq x_v$.

Max-Cut Problem

NP-hard to find the optimal cut.

Max-Cut Problem

NP-hard to find the optimal cut.

However, it is possible to find an **approximately optimal cut** in polynomial time. The Goemans-Williamson algorithm can find a cut that achieves 87.8% of the maximum possible.

Max-Cut Problem

NP-hard to find the optimal cut.

However, it is possible to find an **approximately optimal cut** in polynomial time. The Goemans-Williamson algorithm can find a cut that achieves 87.8% of the maximum possible.

Open question: is there a polynomial-time algorithm that achieves a better approximation of Max-Cut?

Classical-quantum dictionary

Classical CSPS	Quantum Hamiltonians
Variables	Qubits
Constraints	Hamiltonian terms
Assignment	Quantum state
# of satisfied constraints	Energy
Optimal assignment	Ground state

Hamiltonians

Mathematically, a ***n*-qubit Hamiltonian** H is a **Hermitian** n-qubit matrix. It has dimension $2^n \times 2^n$.

Mathematically, a ***n*-qubit Hamiltonian** H is a **Hermitian** n-qubit matrix. It has dimension $2^n \times 2^n$.

By the spectral theorem, we can diagonalize $H = \sum_j E_j \, |v_j\rangle\langle v_j|$.

$\{E_j\}_j$ are the **energy levels** of H. The vector $|v_j\rangle$ is an **energy eigenstate** with energy E_j.

Hamiltonians

The physical interpretation of a Hamiltonian H: it assigns an **average energy** to every n-qubit state $|\psi\rangle$. Energy of $|\psi\rangle$ with respect to H: $\langle\psi| H |\psi\rangle$

Hamiltonians

The physical interpretation of a Hamiltonian H: it assigns an **average energy** to every n-qubit state $|\psi\rangle$. Energy of $|\psi\rangle$ with respect to H: $\langle\psi| H |\psi\rangle$

Since energy eigenstates form a basis, we can write $|\psi\rangle = \sum_j \alpha_j |v_j\rangle$.

Thus energy of $|\psi\rangle = \langle\psi| \left(\sum_j E_j |v_j\rangle\langle v_j| \right) |\psi\rangle$

$= \sum_j E_j |\langle\psi \mid v_j\rangle|^2 = \sum_j E_j |\alpha_j|^2$.

Hamiltonians

The states $|\psi\rangle$ with **minimum energy** with respect to H are called **ground states**. The minimum energy is called **ground energy**.

$E_{ground} = \min_{|\psi\rangle} \langle\psi| H |\psi\rangle$.

Hamiltonians

The states $|\psi\rangle$ with **minimum energy** with respect to H are called **ground states**. The minimum energy is called **ground energy**.

$E_{ground} = \min_{|\psi\rangle} \langle\psi| H |\psi\rangle$.

Exercise: The ground energy of H is equal to the **minimum eigenvalue** of H, and all ground states are eigenvectors of H.

Local Hamiltonians

Physics focuses on **local Hamiltonians**, which means

$$H = H_1 + H_2 + \cdots + H_m$$

where each H_j is a **local Hamiltonian term**, acting nontrivially on a small set of qubits.

Local Hamiltonians

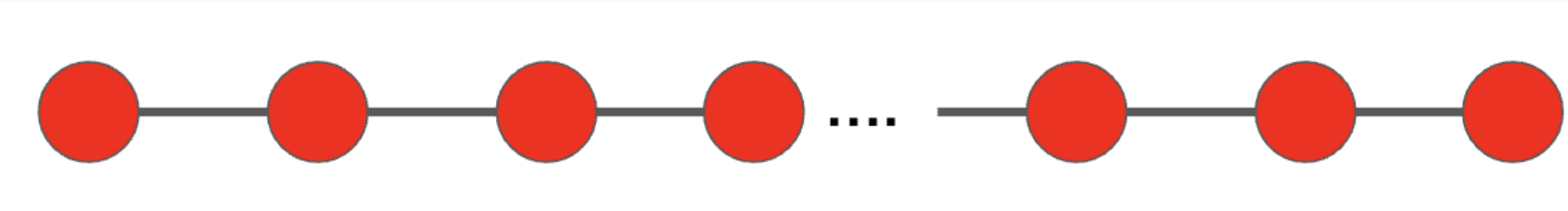
Physics focuses on **local Hamiltonians**, which means

$$H = H_1 + H_2 + \cdots + H_m$$

where each H_j is a **local Hamiltonian term**, acting nontrivially on a small set of qubits.

Just like how quantum circuits consist of **local gates** acting on one or two qubits at a time, the interesting Hamiltonians in physics are built out of local terms.

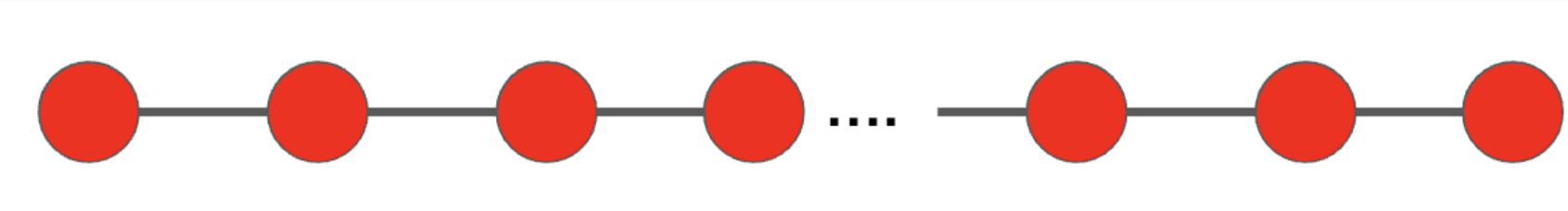
Local Hamiltonians



Example: a line of interacting particles.

Each vertex corresponds to a qubit. Qubits only interact with neighboring qubits.

Local Hamiltonians



Example: a line of interacting particles.

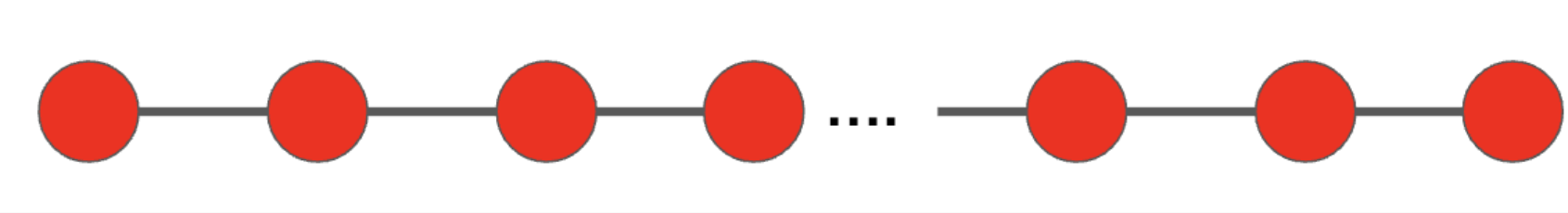
Each vertex corresponds to a qubit. Qubits only interact with neighboring qubits.

For every pair of neighbors $(j, j+1)$, there is a Hamiltonian term

$$H_{j,j+1} = I_{j-1} \otimes h_{j,j+1} \otimes I_{n-j-1}$$

where $h_{j,j+1}$ is a 4×4 Hermitian matrix.

Local Hamiltonians



Example: a line of interacting particles.

The overall Hamiltonian is

$$H = \sum_j H_{j,j+1}$$

Note that H is a **gigantic matrix** $(2^n \times 2^n)$, but it is built out of a small number of local matrices $h_{j,j+1}$. Just like how an n-qubit quantum unitary can be built out of a small number of local unitary gates.

Local Hamiltonians

Local Hamiltonians are prevalent in physics because the laws of nature are inherently local: particles interact with nearby ones.

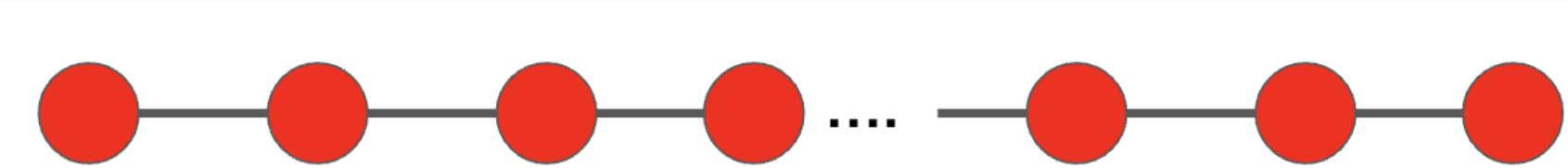
Local Hamiltonians

Local Hamiltonians are prevalent in physics because the laws of nature are inherently local: particles interact with nearby ones.

Depending on what kind of physical phenomena is being investigated, physicists will write down different local Hamiltonians.

For example, electric field, magnetic field, nuclear forces, etc...

Ising Hamiltonian

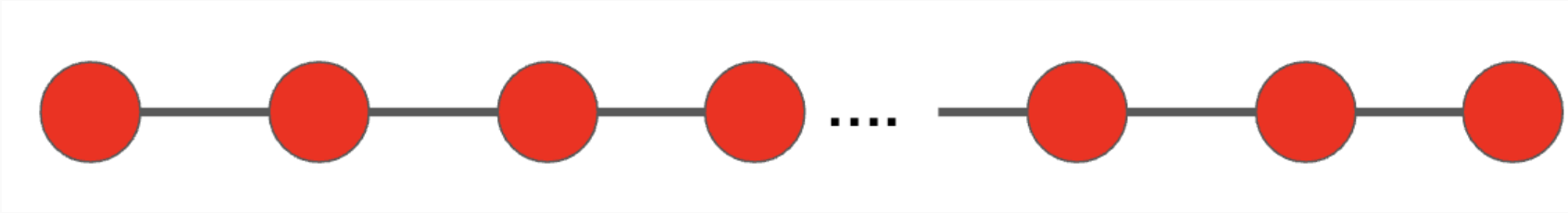


An important model of magnetism in physics.

Each particle is a magnet that points up ($|0\rangle$) or points down ($|1\rangle$). Neighboring magnets want to **anti-align**.

There is also a **global magnetic field** that encourages all magnets to point in a specific direction.

Ising Hamiltonian

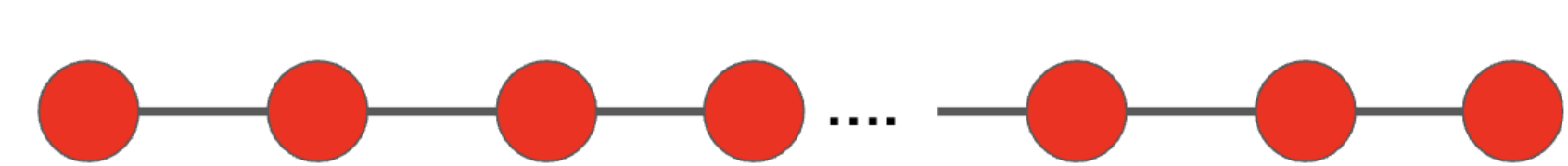


Recall that $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. The **1D Ising Model** is

$$H = \sum_{i=1}^{n-1} Z_i \otimes Z_{i+1} + \mu \sum_{i=1}^{n} Z_i$$

where μ = magnetic field strength parameter.

Ising Hamiltonian



Recall that $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. The **1D Ising Model** is

$$H = \sum_{i=1}^{n-1} Z_i \otimes Z_{i+1} + \mu \sum_{i=1}^{n} Z_i$$

where μ = magnetic field strength parameter.

Note: $Z_i \otimes Z_{i+1}$ and Z_i are implicitly tensored with identity operators on all the other qubits. Each term is a $2^n \times 2^n$ matrix!

Why does μZ_i capture the "global magnetic field" on the i'th qubit?

Why does μZ_i capture the "global magnetic field" on the i'th qubit?

We can diagonalize $Z = |0\rangle\langle 0| - |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$.

Why does μZ_i capture the "global magnetic field" on the i'th qubit?

We can diagonalize $Z = |0\rangle\langle 0| - |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$.

Thus μZ_i has energy μ for any state where i'th qubit is in state $|0\rangle$, and $-\mu$ where i'th qubit is in state $|1\rangle$.

If $\mu > 0$, then i'th qubit "prefers" to be in state $|1\rangle$ (because that's lower energy); otherwise it prefers $|0\rangle$.

Why does $Z_i \otimes Z_{i+1}$ capture the "anti-alignment" interaction between qubits i and $i+1$?

Why does $Z_i \otimes Z_{i+1}$ capture the "anti-alignment" interaction between qubits i and $i+1$?

Its spectral decomposition:

$$Z_i \otimes Z_{i+1} = \Big(|0\rangle\langle 0|_i - |1\rangle\langle 1|_i\Big) \otimes \Big(|0\rangle\langle 0|_{i+1} - |1\rangle\langle 1|_{i+1}\Big)$$
$$= |00\rangle\langle 00|_{i,i+1} + |11\rangle\langle 11|_{i,i+1} - |01\rangle\langle 01|_{i,i+1} - |10\rangle\langle 10|_{i,i+1}$$

Why does $Z_i \otimes Z_{i+1}$ capture the "anti-alignment" interaction between qubits i and $i+1$?

Its spectral decomposition:

$$Z_i \otimes Z_{i+1} = \Big(|0\rangle\langle 0|_i - |1\rangle\langle 1|_i\Big) \otimes \Big(|0\rangle\langle 0|_{i+1} - |1\rangle\langle 1|_{i+1}\Big)$$
$$= |00\rangle\langle 00|_{i,i+1} + |11\rangle\langle 11|_{i,i+1} - |01\rangle\langle 01|_{i,i+1} - |10\rangle\langle 10|_{i,i+1}$$

The lower energy configurations are where qubits i and $i+1$ point in opposite directions!

Ising Hamiltonian

The energy of a state $|\psi\rangle$ in the Ising model is

$$\langle\psi| H |\psi\rangle = \sum_{i=1}^{n-1} \langle\psi| Z_i \otimes Z_{i+1} |\psi\rangle + \mu \sum_{i=1}^{n} \langle\psi| Z_i |\psi\rangle$$

The "anti-alignment" and "global magnetic field" terms **compete** with each other!

Ising Hamiltonian

The energy of a state $|\psi\rangle$ in the Ising model is

$$\langle\psi| H |\psi\rangle = \sum_{i=1}^{n-1} \langle\psi| Z_i \otimes Z_{i+1} |\psi\rangle + \mu \sum_{i=1}^{n} \langle\psi| Z_i |\psi\rangle$$

The "anti-alignment" and "global magnetic field" terms **compete** with each other!

Exercise: what are the minimum energy configurations, depending on μ?

The Ising Hamiltonian is a **classical Hamiltonian**, because it is diagonal in the standard basis. In particular, ground states are all classical basis states.

The Ising Hamiltonian is a **classical Hamiltonian**, because it is diagonal in the standard basis. In particular, ground states are all classical basis states.

An example of a **quantum Hamiltonian** is the **Transverse Field Ising Model**:

$$H = -\sum_{i=1}^{n-1} Z_i \otimes Z_{i+1} + g \sum_{i=1}^{n} X_i$$

where $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.

The Ising Hamiltonian is a **classical Hamiltonian**, because it is diagonal in the standard basis. In particular, ground states are all classical basis states.

An example of a **quantum Hamiltonian** is the **Transverse Field Ising Model**:

$$H = -\sum_{i=1}^{n-1} Z_i \otimes Z_{i+1} + g \sum_{i=1}^{n} X_i$$

where $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.

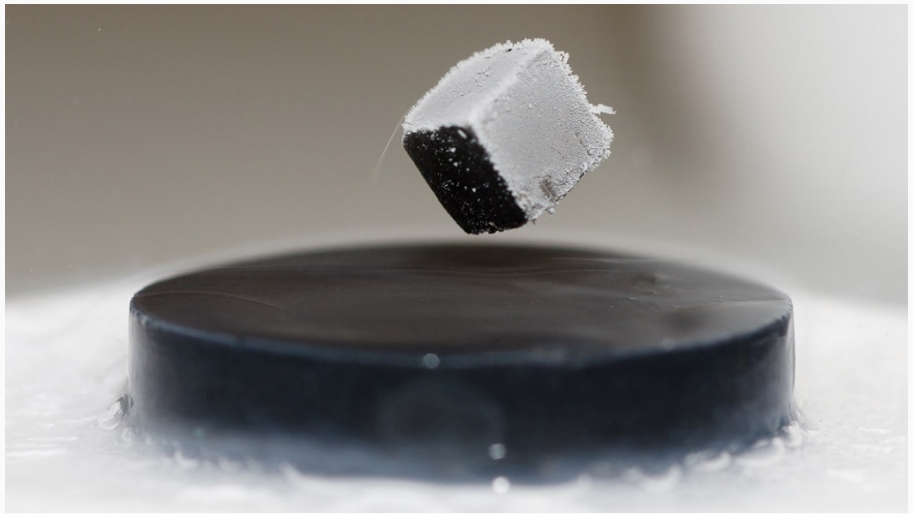
The ground states of this Hamiltonian are generally **entangled and non-classical**.

The important questions: given a (local) Hamiltonian H,

1. What is its ground energy?
2. What are its ground states?
3. How does a quantum system, governed by H, evolve over time?

Ground states

Ground states are interesting because they represent quantum systems at **low temperatures** (e.g. near absolute zero). Ground states of quantum Hamiltonians tend to exhibit bizarre quantum effects.



Ground states

Computing ground states and ground energies of Hamiltonians is not easy!

In fact, it is generally an **NP-hard** problem.

Ground states

Computing ground states and ground energies of Hamiltonians is not easy!

In fact, it is generally an **NP-hard** problem.

Finding ground states of local Hamiltonians is analogous to finding optimal solutions of CSPs.

Next time

Time evolution under a Hamiltonian, and simulating it.