# Simulating Hamiltonian dynamics on a quantum computer

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# Why quantum computing?

**Information is physical.**

**Physics is quantum mechanical.**

In particular: Physical systems are described by vectors in Hilbert space that evolve by unitary transformations and can be measured by projection onto orthogonal subspaces.

# The quantum circuit model

- Start in the state $|0\rangle$
- Apply a sequence of unitary transformations $U_1$, $U_2$, …, $U_k$ chosen from a universal gate set, e.g. {*H*,*T*,CNOT}
- Measure in the computational basis

**But time is not really discrete!**

# Hamiltonian dynamics

Quantum systems evolve according to the Schrödinger equation:

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

$H(t)$ is the **Hamiltonian**.

$H=H^\dagger$ so that the time evolution is *unitary*:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\psi\rangle = i\langle\psi|H^\dagger|\psi\rangle - i\langle\psi|H|\psi\rangle = 0$$

# Solution of Schrödinger equation

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

time independent

*Eigenstates* of $H$: $H\,|\phi_j\rangle = E_j\,|\phi_j\rangle$

$H = \sum_j E_j\,|\phi_j\rangle\langle\phi_j|$ $\quad$ $E_j \in \mathbb{R}$ since $H=H^\dagger$

Suppose $|\psi(0)\rangle = |\phi_j\rangle$

Then $|\psi(t)\rangle = \exp(-i\,E_j\,t)\,|\phi_j\rangle$

Expand a general initial state: $|\psi(0)\rangle = \sum_j c_j\,|\phi_j\rangle$

$|\psi(t)\rangle = \sum_j c_j \exp(-i\,E_j\,t)\,|\phi_j\rangle = U(t)\,|\psi(0)\rangle$

where $U(t) = \exp(-i\,H\,t) = \sum_j (-i\,H\,t)^j / j!$

# Solution of Schrödinger equation

## Time dependent case

$$|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$$

where $U(t) = \mathrm{T}\exp[-i\int_0^t d\tau\, H(\tau)]$

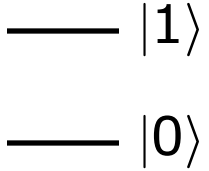
time ordering operator

Special case: Suppose $H(t)$ changes very slowly. Then the evolution is much simpler because of the *Adiabatic Theorem*. More on this later.

# Relation to the circuit model

Unitary quantum gates arise from Hamiltonian dynamics.

**Simple example:** Two level atom.




Apply a laser pulse. $H = \omega \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

$$U(t) = e^{-iHt} = \begin{pmatrix} \cos\omega t & \sin\omega t \\ -\sin\omega t & \cos\omega t \end{pmatrix}$$

$$U(\pi/4\omega) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

But perhaps we can use *many-body* Hamiltonians to perform interesting computations.

# Why consider Hamiltonians?

Simulating physical systems

New kinds of quantum algorithms

- Quantum walks
- Adiabatic quantum computation

Quantum analogue of the Cook-Levin Theorem (Kitaev: "LOCAL HAMILTONIAN is QMA-complete")

# Efficiently realizable Hamiltonians

How do we know what Hamiltonians are legal for use in computations?

**Example:**

Let $x$ = instance of a hard problem

Let $s_x$ = solution of $x$

The Hamiltonian

$$H = \sum_x (|0, s_x\rangle\langle x, 0| + |x, 0\rangle\langle 0, s_x|)$$

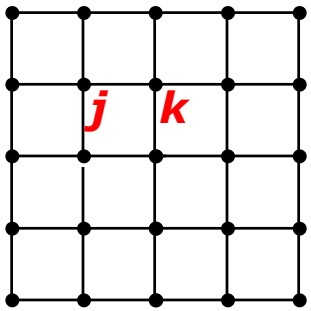
seems hard to implement!

# Efficiently realizable Hamiltonians

Two notions of efficient realizability:

**1.** *H* is the Hamiltonian of a physical system we can "easily" build

Spins arranged on a 2D lattice




$$H = \sum_{j,k} a_{jk}\, \sigma_z^{(j)} \sigma_z^{(k)} + \sum_j b_j\, \sigma_x^{(j)}$$

where $a_{jk}$=0 for non-adjacent sites

# Efficiently realizable Hamiltonians

Two notions of efficient realizability:

**2.** $H$ is a Hamiltonian that can be efficiently simulated in the circuit model

**Def.** A Hamiltonian $H$ acting on $n$ qubits can be *efficiently simulated* if for any $\varepsilon>0$, $t>0$ there is a quantum circuit $U$ consisting of poly($n$,$t$,$1/\varepsilon$) gates such that $\|U - e^{-iHt}\|<\varepsilon$.

Note: This will include the "physically reasonable" Hamiltonians.

# Tools for simulating Hamiltonians

**Rule 1.** Local Hamiltonians.

If $H$ acts on $O(1)$ qubits, it can be efficiently simulated.

**Rule 2.** Rescaling.

If $H$ can be efficiently simulated, then $cH$ can be efficiently simulated for any $c=\text{poly}(n)$.

# Tools for simulating Hamiltonians

**Rule 3.** Linear combination.

If $H_j$ can be efficiently simulated, then $\sum_j H_j$ can be efficiently simulated.

**Lemma.** Lie product formula.

Let $h = \max_j \|H_j\|$. Then

$$e^{-i(H_1+\cdots+H_k)t} = (e^{-iH_1 t/r} \ldots e^{-iH_k t/r})^r + O\left(\frac{kh^2t^2}{r}\right)$$

# Lie product formula

**Proof.**

By Taylor expansion,

$$e^{-iHt/r} = 1 - iHt/r + O(h^2t^2/r^2)$$

Thus

$$\begin{aligned}
&(e^{-iH_1t/r} \dots e^{-iH_kt/r})^r \\
&\quad = [1 - i(H_1 + \cdots + H_k)t/r + O(kh^2t^2/r^2)]^r \\
&\quad = [e^{-i(H_1+\cdots+H_k)t/r} + O(kh^2t^2/r^2)]^r \\
&\quad = e^{-i(H_1+\cdots+H_k)t} + O(kh^2t^2/r)
\end{aligned}$$

□

# The story so far

Using Rules 1,2,3 we can simulate many "physical" Hamiltonians.

*H* = sum of terms, each acting on a constant number of qubits

Recall example of a spin glass:

$$H = \sum_{j,k} a_{jk}\, \sigma_z^{(j)} \sigma_z^{(k)} + \sum_j b_j\, \sigma_x^{(j)}$$

Lloyd 96

# Tools for simulating Hamiltonians

**Rule 4.** Commutation.

If $H_1$, $H_2$ can be efficiently simulated, then $i[H_1,H_2]$ can be efficiently simulated.

**Rule 5.** Unitary conjugation.

If $H$ can be efficiently simulated and the unitary operation $U$ can be efficiently implemented, then $U^\dagger HU$ can be efficiently simulated.

**Proof.** $e^{-iU^\dagger HUt} = U^\dagger e^{-iHt} U$ □

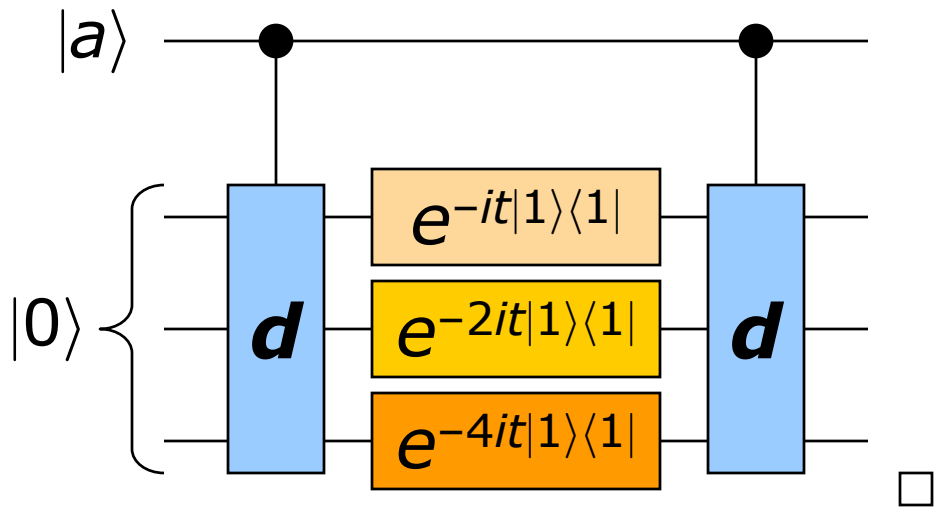
# Tools for simulating Hamiltonians

**Rule 6.** Computable phase shifts.

If $H$ is diagonal and the diagonal element $d(a)=\langle a|H|a\rangle$ can be efficiently computed for any $a$, then $H$ can be efficiently simulated.

**Proof.**

$$|a,0\rangle \rightarrow |a,d(a)\rangle$$
$$\rightarrow e^{-itd(a)}|a,d(a)\rangle$$
$$\rightarrow e^{-itd(a)}|a,0\rangle$$




□

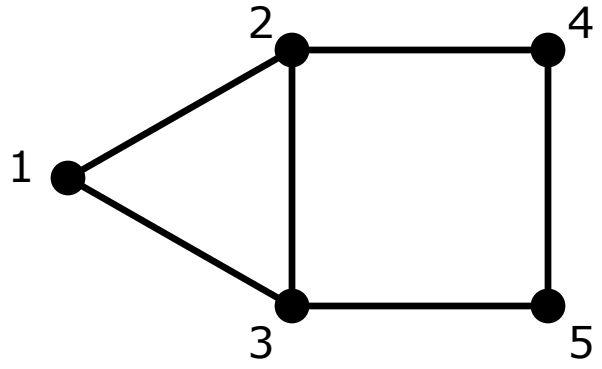
# Tools for simulating Hamiltonians

**Rule 7.** Sparse Hamiltonians.

Suppose that for any $a$, one can efficiently compute all the values of $b$ for which $\langle a|H|b\rangle$ is nonzero. Then $H$ can be efficiently simulated.

**Example:**

$$H = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$



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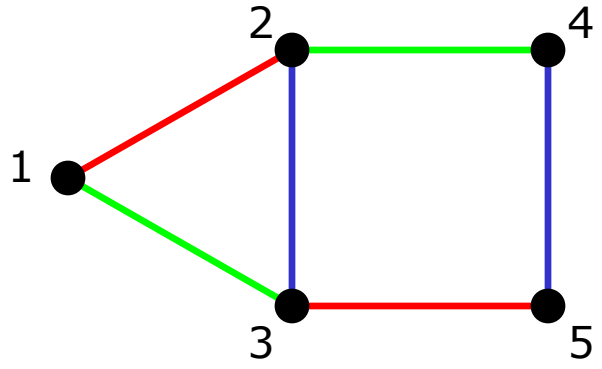

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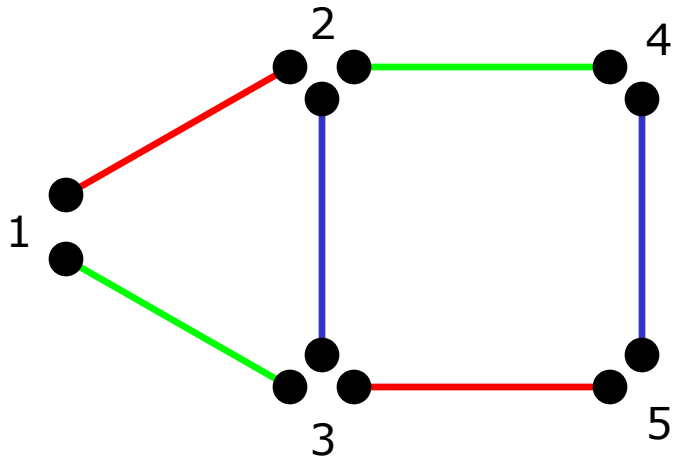

# Coloring a sparse graph

**Lemma.**

Given an undirected graph $G$ with $N$ vertices and maximum degree $d$, suppose one can efficiently compute the neighbors of a given vertex. Then there is an efficiently computable function $c(a,b)=c(b,a)$ taking $O(d^2 \log^2 N)$ values such that for all $a$, $c(a,b)=c(a,b')$ implies $b=b'$.

Aharonov, Ta-Shma 03

# Coloring a sparse graph

**Proof.**

Let index($a$,$b$) be the index of $b$ in the list of neighbors of $a$.

Let $k(a,b)$ be the smallest $k$ such that $a \neq b \pmod{k}$.
Note $k(a,b)=k(b,a)$ and $k=O(\log N)$.

For $a<b$, define

$c(a,b) := (\text{index}(a,b), \text{index}(b,a), k(a,b), b \bmod k(a,b))$

For $a>b$, define $c(a,b) := c(b,a)$.

Suppose $c(a,b)=c(a,b')$. Four cases:

**i.** $a<b$, $a<b'$. index($a$,$b$)=index($a$,$b'$) $\Rightarrow$ $b=b'$.

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**ii.** $a>b$, $a>b'$. $\text{index}(a,b)=\text{index}(a,b') \Rightarrow b=b'$.

**iii.** $a<b$, $a>b'$. $k(a,b)=k(a,b')$, $a=b \bmod k$, contradiction.

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**iii.** $a<b$, $a>b'$. $k(a,b)=k(a,b')$, $a=b \bmod k$, contradiction.

**iv.** $a>b$, $a<b'$. $k(a,b)=k(a,b')$, $a=b' \bmod k$, contradiction.

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**iv.** $a>b$, $a<b'$. $k(a,b)=k(a,b')$, $a=b' \bmod k$, contradiction. □

# Simulating a sparse Hamiltonian

**Proof.** (of Rule 7)

Write $H$ as a diagonal matrix plus a matrix with zeros on the diagonal. The diagonal part can be simulated using Rule 6 and combined with the off-diagonal piece using Rule 3. Thus assume $H$ has zeros on the diagonal WLOG.

Let $v_c(a)$ be the vertex connected to $a$ by an edge of color $c$.

Let $x_c(a) := \mathrm{Re}\ \langle a|H|v_c(a)\rangle$, $y_c(a) := \mathrm{Im}\ \langle a|H|v_c(a)\rangle$.

Consider the state space $|a,b,z\rangle$ where vertices are $|a,0,0\rangle$.

We can efficiently implement unitary operators

$$V_c\,|a,0,0\rangle = |a,\ v_c(a),\ x_c(a)\rangle$$
$$W_c\,|a,0,0\rangle = |a,\ v_c(a),\ y_c(a)\rangle.$$

(If no such vertex, $v_c(a)=11\ldots1$, $x_c(a)=y_c(a)=0$.)

We can efficiently simulate the Hamiltonians

$$S\,|a,b,x\rangle = x\,|b,a,x\rangle$$
$$T\,|a,b,y\rangle = i\,y\,|b,a,-y\rangle$$

using Rules 1,5,6.

# Simulating a sparse Hamiltonian

**Proof.** (of Rule 7, continued)

Using Rules 3,5 we can efficiently simulate

$$\tilde{H} = \sum_c (V_c^\dagger S V_c + W_c^\dagger T W_c).$$

This has the proper action on vertices:

$$\begin{aligned}
\tilde{H}|a,0,0\rangle &= \sum_c [V_c^\dagger S|a, v_c(a), x_c(a)\rangle \\
&\qquad + W_c^\dagger T|a, v_c(a), y_c(a)\rangle] \\
&= \sum_c [x_c(a)\, V_c^\dagger|v_c(a), a, x_c(a)\rangle \\
&\qquad + i y_c(a)\, W_c^\dagger|a, v_c(a), -y_c(a)\rangle] \\
&= \sum_c [x_c(a) + i y_c(a)]|v_c(a), 0, 0\rangle \qquad \square
\end{aligned}$$

# Example: Particle in a potential

Consider the Hamiltonian

$$H = \frac{p^2}{2m} + V(x)\,, \qquad p^2 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

Lattice version (lattice spacing *l*):

$$p^2|x\rangle = \tfrac{1}{l^2}(2|x\rangle - |x+1\rangle - |x-1\rangle)$$

$p^2$ is diagonal in the Fourier basis, and the unitary operator corresponding to the Fourier transform is efficiently implementable, so H can be simulated using Rules 3,5,6.

Alternatively, just note that H is sparse and computable, so Rule 7 applies.

Wiesner 96, Zalka 98

# Summary

Quantum systems evolve according to the Schrödinger equation $i\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H(t)|\psi(t)\rangle$

Such systems can be efficiently simulated by a universal quantum computer when *H*

- Is a sum of terms, each acting on at most a constant number of qubits (Rule 1,2,3)
- Is *i* times the commutator of two simulable Hamiltonians (Rule 4)
- Differs from a simulable Hamiltonian by an efficiently implementable unitary transformation (Rule 5)
- Is sparse and efficiently computable (Rules 6,7)

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Hamiltonian dynamics in quantum algorithms:
See next lecture