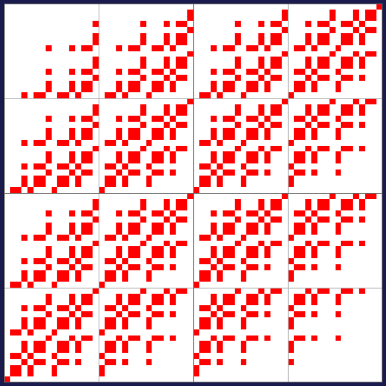
My computer wants to be quantum (when it grows up)

A tutorial on classical simulation of quantum computers



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What shall we talk about?

Seducing Nature into doing our work

Someone's crisis is another guy's opportunity

Not up or down, but up *and* down

The astonishing power of combinatorics

The Matrix is your friend *(take the quantum pill)*

Sorting your life priorities is NP-hard

In order to compute, do not wake up the dragon

Seducing Nature into doing our work

Optimization problems:

- Traveling salesman problem (TSP), knapsack problem...
- Factorizing: Minimize $E(x, y) = |N - xy|$.

Nature Optimizes:

- E.g., crystal structure *minimizes* the energy, and solves a tough problem.

Complexity classes:

- **P** problems: can be solved in polynomial time.
- **NP** problems: can be checked in polynomial time.

The dimensionality curse

CLASSICAL vs QUANTUM: **information content of a state**.

Consider space divided into N boxes.

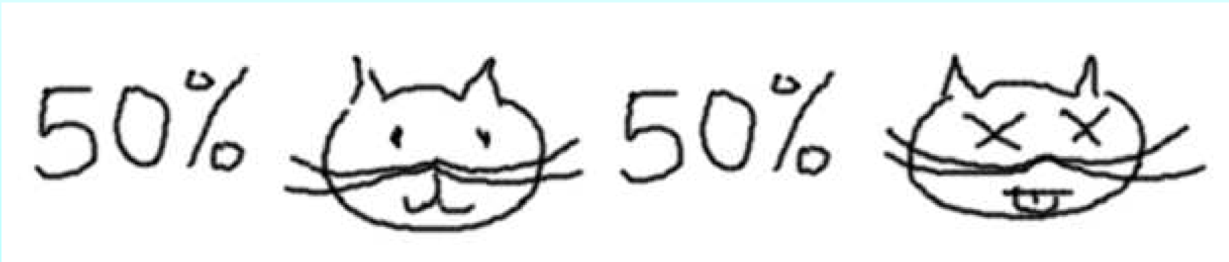
CLASSICAL DESCRIPTION: Select one configuration in $\{0,1\}^N$.

QUANTUM DESCRIPTION: Map $\psi : \{0,1\}^N \mapsto \mathbb{C}$.

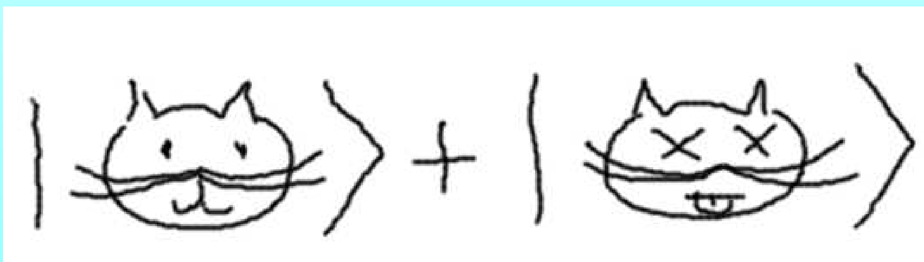
Configuration	CLASSICAL	QUANTUM
000	-	$+1/2$
001	-	0
010	-	$-1/2$
011	-	$+1/2$
100	-	0
101	•	$-1/2$
110	-	0
111	-	0

Richard Feynman: Turn the crisis into an opportunity!

Brave Quantum World



Probabilistic or mixed state



Pure state or *ket*

Brave Quantum World

$$|\uparrow\rangle + |\downarrow\rangle = |\rightarrow\rangle$$

Measurements of S^x are **certain**.

Brave Quantum World

General Qubit

$$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$$

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

Probability for up: $|\alpha|^2$, **Probability for down:** $|\beta|^2$

$$|\alpha|^2 + |\beta|^2 = 1$$

General Quantum State

$$|\psi\rangle = \sum_{i=1}^{N} \alpha_i |s_i\rangle$$

Probability for i-th state: $|\alpha_i|^2$, $\quad \sum_{i=1}^{N} |\alpha_i|^2 = 1.$

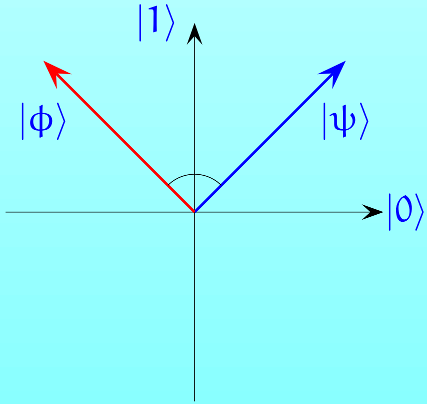
States as Vectors

- **General Qubit:**

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \qquad \Longrightarrow \qquad \psi = (\alpha, \beta)$$

- **General Quantum State:**

$$|\psi\rangle = \sum_{i=1}^{N} \alpha_i |s_i\rangle, \qquad \Longrightarrow \qquad \psi = (\alpha_1, \alpha_2, \ldots, \alpha_N)$$



Probability of mistaking

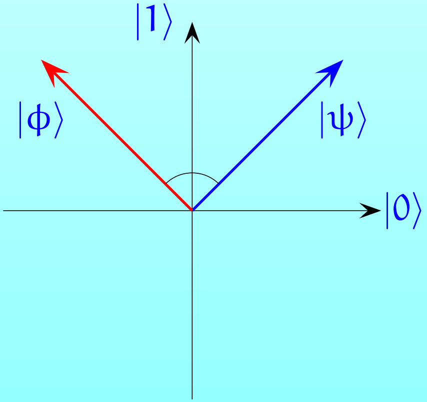
- Two quantum states,

$$|\psi\rangle = \psi_0|0\rangle + \psi_1|1\rangle, \qquad |\phi\rangle = \phi_0|0\rangle + \phi_1|1\rangle$$

$$\psi = (\psi_0, \psi_1), \qquad \phi = (\phi_0, \phi_1)$$

- To compute the probability of **mistaking** them:

$$\text{Prob}(\phi, \psi) = \cos^2(\phi, \psi)$$
$$= (\bar{\phi}_0\psi_0 + \bar{\phi}_1\psi_1)^2$$
$$\equiv |\langle\phi|\psi\rangle|^2$$



Each state is a *direction*: you can not mistake N and E, but you *can* mistake N and NE.

Probability of mistaking

- E.g. what is the probability of mistaking $|{\rightarrow}\rangle$ and $|{\uparrow}\rangle$?

$$|{\rightarrow}\rangle = \frac{1}{\sqrt{2}}\left(|{\uparrow}\rangle + |{\downarrow}\rangle\right) = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)$$

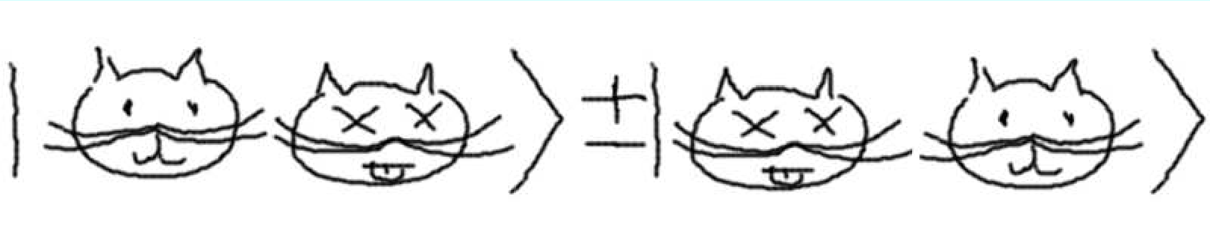
$$|{\uparrow}\rangle = (1, 0)$$

$$\text{Prob}(\rightarrow, \uparrow) = |\langle \rightarrow \mid \uparrow \rangle|^2 = \left|\frac{1}{\sqrt{2}} \cdot 1 + \frac{1}{\sqrt{2}} \cdot 0\right|^2 = \frac{1}{2}$$

Many-cat Theory

- What if we have two killer cats?

- Why not in a linear superposition?



Many-cat Theory

- Tensor basis for two qubits:

$$\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$$

- Generic state:

$$|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$$

$$\psi = (\alpha, \beta, \gamma, \delta)$$

- We need to store $4 = 2^2$ numbers.

- Specially relevant state is the Einstein-Podolsky-Rosen (EPR):

$$|S\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right), \qquad S = \left(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right)$$

Many-cat Theory

- What about states like

$$|\psi\rangle = |\rightarrow\rightarrow\rangle$$

- Introduce the **tensor product**, $\otimes$, which works like a product!

$$|\psi\rangle = |\rightarrow\rangle \otimes |\rightarrow\rangle$$

$$= \left(\frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)\right)$$

$$= \frac{1}{2}\left(|\uparrow\rangle \otimes |\uparrow\rangle + |\uparrow\rangle \otimes |\downarrow\rangle + |\downarrow\rangle \otimes |\uparrow\rangle + |\downarrow\rangle \otimes |\downarrow\rangle\right)$$

$$= \frac{1}{2}\left(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle\right)$$

$$\psi = \frac{1}{2}(1, 1, 1, 1)$$

Many-cat Theory

- Tensor basis for *three* qubits:

$$\{|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle\}$$

- Generic state:

$$|\psi\rangle = \alpha|000\rangle + \beta|001\rangle + \gamma|010\rangle + \delta|011\rangle + \epsilon|100\rangle + \zeta|101\rangle + \eta|110\rangle + \theta|111\rangle$$

$$\psi = (\alpha, \beta, \gamma, \delta, \epsilon, \zeta, \eta, \theta)$$

- We need to store $8 = 2^3$ numbers.

- For N qubits, we need to store 2^N numbers! **The dimensionality curse!**

Many-cat Theory

- Some special many-qubit states: GHZ, Néel & Dicke.

$$|\mathrm{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\cdots\rangle + |111\cdots\rangle)$$

$$|N\rangle = \frac{1}{\sqrt{2}}(|1010\cdots\rangle + |0101\cdots\rangle)$$

$$|D_{4,2}\rangle = \frac{1}{\sqrt{6}}(|0011\rangle + |0101\rangle + |0110\rangle + |1001\rangle + |1010\rangle + |1100\rangle)$$

$$D_{4,2} = (0,0,0,1,0,1,1,0,0,1,1,0,1,0,0,0)$$

- Do you observe a link between many-qubit states and formal languages?

Formal language: $\{0,1\}^* \mapsto \{0,1\}$,

Many-qubit state: $\{0,1\}^N \mapsto \mathbb{C}$.

Qubism

- Our group developed a plotting scheme for many-qubit states.

00 → Upper left 01 → Upper right
10 → Lower left 11 → Lower right

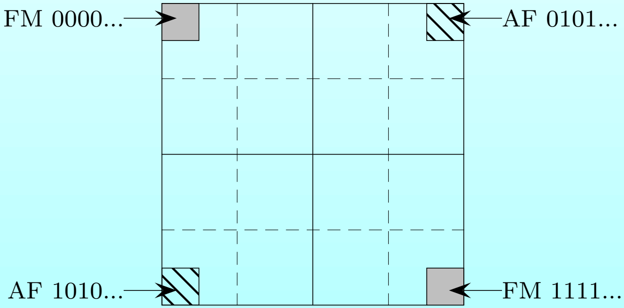
Level 1
2 qubits

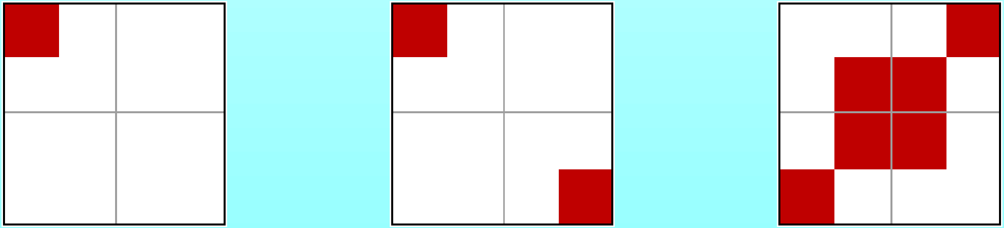
00	01
10	11

Level 2
4 qubits

0000	0001	0100	0101
0010	0011	0110	0111
1000	1001	1100	1101
1010	1011	1110	1111

Qubism

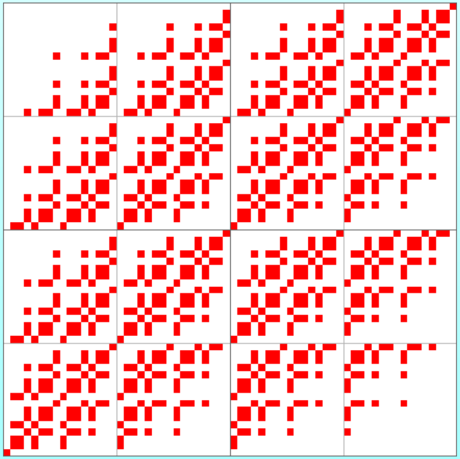




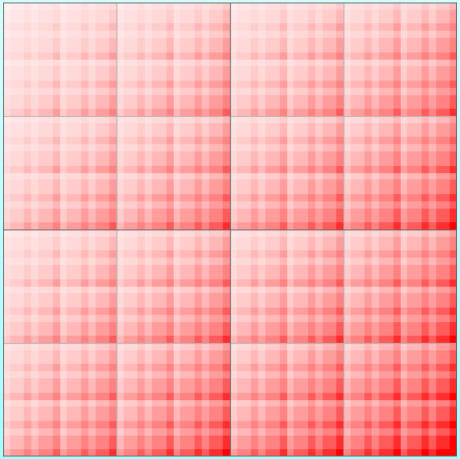
$|0000\rangle$ $|GHZ\rangle$ $|D_{4,2}\rangle$

Qubism

- Qubistic plots are typically *fractal*



$|D_{12,6}\rangle$



$(\alpha|0\rangle + \beta|1\rangle)^{\otimes 12}$

Energy

- The dynamics is specified if we know the energy of all states.
- First example, external magnetic field: $E = \Gamma S^z$.

$$|\uparrow\rangle \quad \rightarrow \quad E = \Gamma, \qquad\qquad |\downarrow\rangle \quad \rightarrow \quad E = -\Gamma$$

- What is the energy of $|\rightarrow\rangle$? A random variable!
- OK, what is the *expected* energy of $|\rightarrow\rangle$?

$$\begin{aligned}\langle E \rangle &= p(\uparrow) \cdot E(\uparrow) + p(\downarrow) \cdot E(\downarrow) \\ &= \frac{1}{2} \cdot \Gamma + \frac{1}{2} \cdot (-\Gamma) = 0\end{aligned}$$

- And for a generic qubit $|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$?

$$\begin{aligned}\langle E \rangle &= p(\uparrow) \cdot E(\uparrow) + p(\downarrow) \cdot E(\downarrow) \\ &= |\alpha|^2 \cdot \Gamma + |\beta|^2 \cdot (-\Gamma) \\ &= \Gamma \left(|\alpha|^2 - |\beta|^2 \right)\end{aligned}$$

Enter The Matrix

- Each observable can be associated to a linear operator (=matrix);

$$S^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad S^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

- Expected values on state $|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$,

$$\langle\psi|S^z|\psi\rangle = (\bar{\alpha}, \bar{\beta}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = (\bar{\alpha}, \bar{\beta}) \begin{pmatrix} \alpha \\ -\beta \end{pmatrix} = |\alpha|^2 - |\beta|^2$$

$$\langle\psi|S^x|\psi\rangle = (\bar{\alpha}, \bar{\beta}) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = (\bar{\alpha}, \bar{\beta}) \begin{pmatrix} \beta \\ \alpha \end{pmatrix} = \bar{\alpha}\beta + \alpha\bar{\beta}$$

- The matrix corresponding to the *energy* is called **Hamiltonian**.

Enter The Matrix

- Each matrix has some specially dear states, called **eigenstates**.

$$H|\varphi\rangle = E|\varphi\rangle$$

- Eigenvector: $|\varphi\rangle$; Eigenvalue: E.
- Example, S^z:

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = (+1)\cdot\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = (-1)\cdot\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$S^z|\uparrow\rangle = (+1)|\uparrow\rangle, \qquad S^z|\downarrow\rangle = (-1)|\downarrow\rangle$$

- Example, S^x:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = (+1)\cdot\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = (-1)\cdot\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$S^x|\rightarrow\rangle = (+1)|\rightarrow\rangle, \qquad S^x|\leftarrow\rangle = (-1)|\leftarrow\rangle$$

Enter The Matrix

- A symmetric matrix $N \times N$ has N orthogonal eigenstates:

$$H|\varphi_i\rangle = E_i|\varphi_i\rangle, \qquad \{|\varphi_i\rangle, E_i\}$$

$$\langle\varphi_i|\varphi_j\rangle = \delta_{ij}.$$

- Finding eigenstates and eigenvalues (diagonalization) is efficient, $O(N^3)$.
- On $|\psi\rangle$, measurement of energy will yield one of the E_i, *randomly*.
- Probability for outcome E_i = probability of mistaking $|\psi\rangle$ and $|\varphi_i\rangle$.

$$p(E_i) = |\langle\varphi_i|\psi\rangle|^2$$

- Eigenvalues are ordered: $E_1 < E_2 < \cdots < E_N$.
- The minimal possible energy is E_1 for $|\varphi_1\rangle$, the **Ground State**.

Many-body Hamiltonians

- Recipe: Find out how H acts on all basis states.
- Elements of the game:

$$S^z|0\rangle = -|0\rangle, \quad S^z|1\rangle = |1\rangle; \qquad S^x|0\rangle = |1\rangle, \quad S^x|1\rangle = |0\rangle$$

- Example, $H = S_1^z + S_2^x$

$$\begin{aligned}
(S_1^z + S_2^x)\,|00\rangle &= -|00\rangle + |01\rangle = (-1,+1,0,0),\\
(S_1^z + S_2^x)\,|01\rangle &= -|01\rangle + |00\rangle = (+1,-1,0,0),\\
(S_1^z + S_2^x)\,|10\rangle &= +|10\rangle + |11\rangle = (0,0,+1,+1),\\
(S_1^z + S_2^x)\,|11\rangle &= +|11\rangle + |10\rangle = (0,0,+1,+1),
\end{aligned}$$

$$H = S_1^z + S_2^z = \begin{pmatrix} -1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

Many-body Hamiltonians

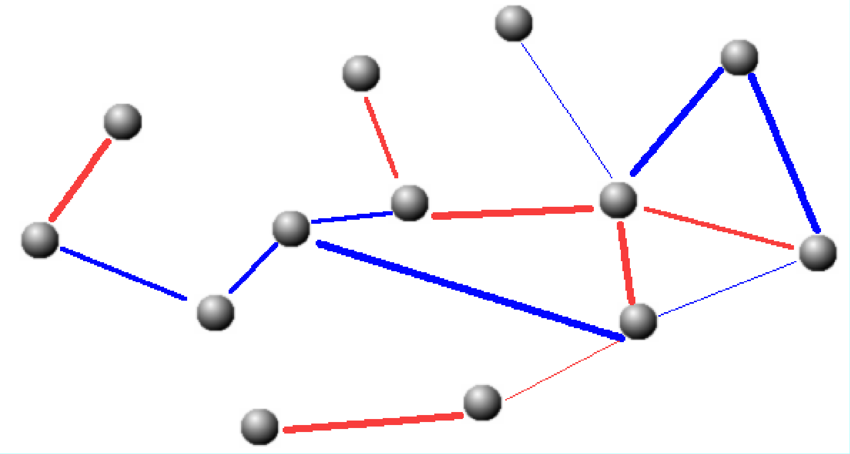
- Another example, $H = S_1^x S_2^x$

$$
\begin{aligned}
S_1^x S_2^x |00\rangle &= |11\rangle = (0,0,0,1),\\
S_1^x S_2^x |01\rangle &= |10\rangle = (0,0,1,0),\\
S_1^x S_2^x |10\rangle &= |01\rangle = (0,1,0,0),\\
S_1^x S_2^x |11\rangle &= |00\rangle = (1,0,0,0).
\end{aligned}
$$

$$
H = S_1^x S_2^x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}
$$

The Spin-Glass Problem

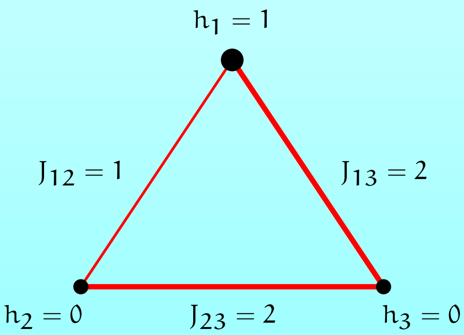
- Draw a graph with your life aims.



The Spin-Glass Problem

- Ising spin-glass model:

$$H_I = \sum_{\langle i,j \rangle} J_{ij}\, S_i^z S_j^z + \sum_i h_i\, S_i^z$$



$$H_I|000\rangle = (1 + 2 + 2 - 1)|000\rangle = +4|000\rangle,$$

$$H_I|001\rangle = (1 - 2 - 2 - 1)|001\rangle = -4|001\rangle,$$

$$H_I|010\rangle = (-1 + 2 - 2 - 1)|010\rangle = -2|010\rangle,$$

$$H_I|011\rangle = (-1 - 2 + 2 - 1)|011\rangle = -2|011\rangle,$$

$$H_I|100\rangle = (-1 - 2 + 2 + 1)|100\rangle = +0|100\rangle,$$

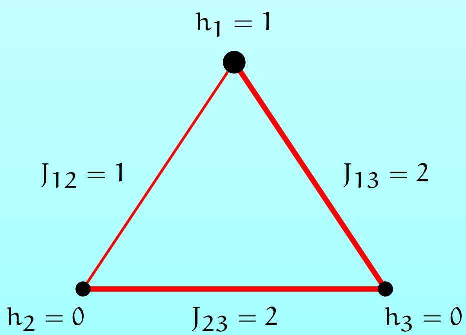
$$H_I|101\rangle = (-1 + 2 - 2 + 1)|101\rangle = +0|101\rangle,$$

$$H_I|110\rangle = (+1 - 2 - 2 + 1)|110\rangle = -2|110\rangle,$$

$$H_I|111\rangle = (+1 + 2 + 2 + 1)|111\rangle = 6|111\rangle.$$

The Spin-Glass Problem

$$H_I = \sum_{\langle i,j \rangle} J_{ij}\, S_i^z S_j^z + \sum_i h_i\, S_i^z$$



$$H_I = \begin{pmatrix} +4 & & & & & & & \\ & -4 & & & & & & \\ & & -2 & & & & & \\ & & & -2 & & & & \\ & & & & 0 & & & \\ & & & & & 0 & & \\ & & & & & & -2 & \\ & & & & & & & +6 \end{pmatrix}$$

- The **Ground State** of H_I is the solution to an **NP**-complete problem!
- But... how to cool the system down? System is **glassy**!

Transverse Field

- The effect of a S^x external field is to *flip* the spin!

$$H_X = -\sum_i S_i^x,$$

- Ground State is the *democratic state*:

$$|\varphi_1\rangle = |\rightarrow\rangle^{\otimes N}$$

$$= \frac{1}{\sqrt{8}}\left(|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle + |111\rangle\right)$$

Transverse Field

$$(S_1^x + S_2^x + S_3^x)\,|000\rangle = |100\rangle + |010\rangle + |001\rangle,$$

$$(S_1^x + S_2^x + S_3^x)\,|001\rangle = |101\rangle + |011\rangle + |000\rangle,$$

$$(S_1^x + S_2^x + S_3^x)\,|010\rangle = |110\rangle + |000\rangle + |011\rangle,$$

$$(S_1^x + S_2^x + S_3^x)\,|011\rangle = |111\rangle + |001\rangle + |010\rangle,$$

$$(S_1^x + S_2^x + S_3^x)\,|100\rangle = |000\rangle + |110\rangle + |101\rangle,$$

$$(S_1^x + S_2^x + S_3^x)\,|101\rangle = |001\rangle + |111\rangle + |100\rangle,$$

$$(S_1^x + S_2^x + S_3^x)\,|110\rangle = |010\rangle + |100\rangle + |111\rangle,$$

$$(S_1^x + S_2^x + S_3^x)\,|111\rangle = |011\rangle + |101\rangle + |110\rangle.$$

$$H_X = -\begin{pmatrix} & 1 & 1 & & 1 & & & \\ 1 & & & 1 & & 1 & & \\ 1 & & & 1 & & & 1 & \\ & 1 & 1 & & & & 1 & 1 \\ 1 & & & & & 1 & & \\ & 1 & & & 1 & & & 1 \\ & & 1 & & 1 & & & 1 \\ & & & 1 & & 1 & 1 & \end{pmatrix}$$

Adiabatic Quantum Computation

1.- Build a tunable machine, with Hamiltonian

$$H(s) = s\,H_I + (1-s)\,H_X$$

2.- Start with $s = 0$, get the GS of H_X (easy!).

3.- Increase s with care! (Don't wake the dragon!)

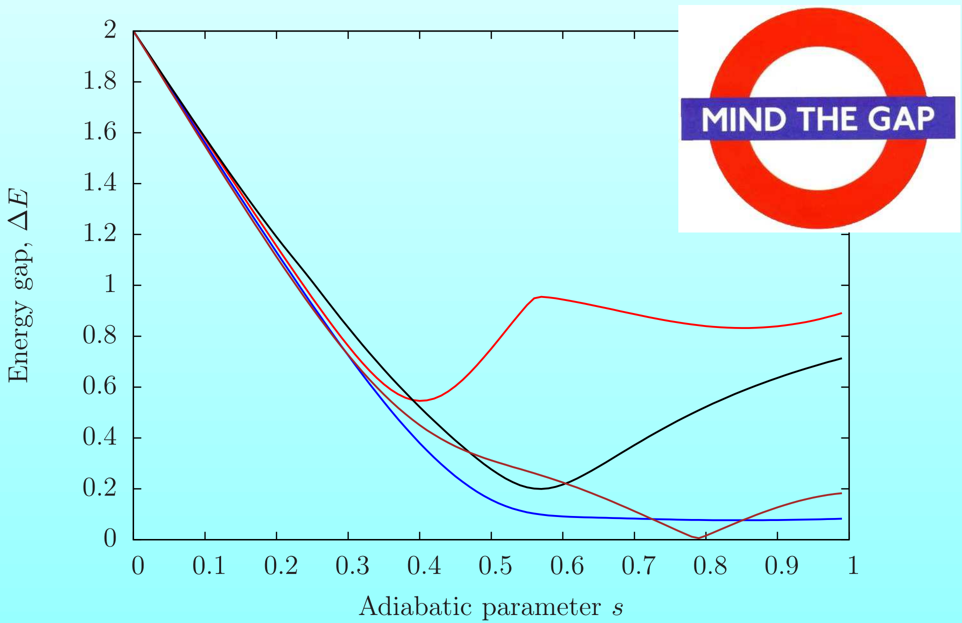
4.- When $s = 1$, read the solution: just measure S^z on each qubit.

- How fast can we get? Landau-Zener formula.

$$\nu \propto (\Delta E)^2 = (E_2 - E_1)^2$$

$$T_{AQC} \propto \int_0^1 \frac{ds}{(E_2(s) - E_1(s))^2}$$

Mind the Gap



MIND THE GAP
Energy gap, ΔE
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
Adiabatic parameter s

Now, let's play!

- Connect to `http://github.com/jvrlag/qtoys`
- Download `Qtoys`, it is GPL-free.
- Follow the compilation instructions (for Linux), or translate to your pet system.
- Run `xqshow`, if possible with some smooth jazz.
- Open the code, change it freely, play.
- If you get to publish a paper, buy me a beer! :)

Thank you for your Attention!

- Visit our bar: `http://mononoke.fisfun.uned.es/jrlaguna`
- Remember the main web: `http://github.com/jvrlag/qtoys`

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