Quantum Hamiltonian Complexity

Part I

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Postulate of Quantum Mechanics - Measurement

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Hermitian Operator with:
Eigenvalues: $\lambda_0, \ldots, \lambda_{N-1}$
Eigenvectors: $|v_0\rangle, \ldots, |v_{N-1}\rangle$

Measurement, cont.

State: $|\Phi\rangle$

Measure quantity - operator A = $\sum_i \lambda_i |v_i\rangle\langle v_i|$

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$|\Phi\rangle = \alpha_0|v_0\rangle + \cdots + \alpha_{N-1}|v_{N-1}\rangle$

Probability of outcome λ_i is:

$$|\alpha_i|^2 = |\langle v_i|\Phi\rangle|^2 = \langle\Phi|v_i\rangle\langle v_i|\Phi\rangle$$

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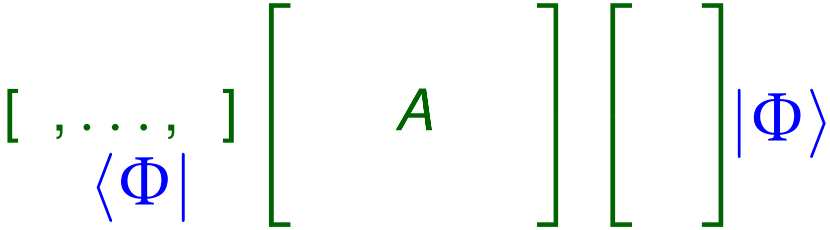

The Hamiltonian Operator - dynamics

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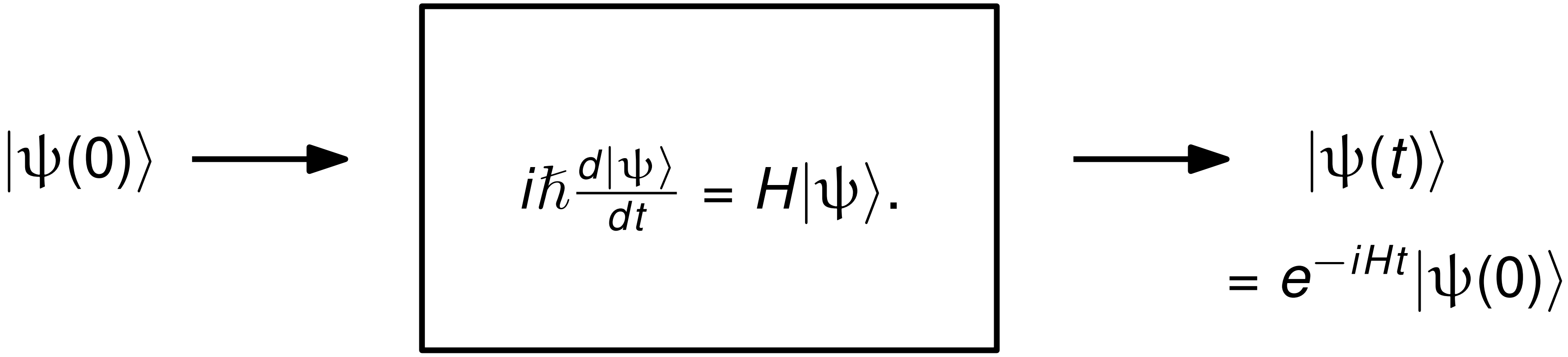

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$$\rho_{eq} = \frac{e^{-\beta H}}{Z} \quad \text{where} \quad Z = \mathrm{Tr}\left(e^{-\beta H} \right)$$

[Linden, Popescu, Short, Winter arXiv:0812.2385]

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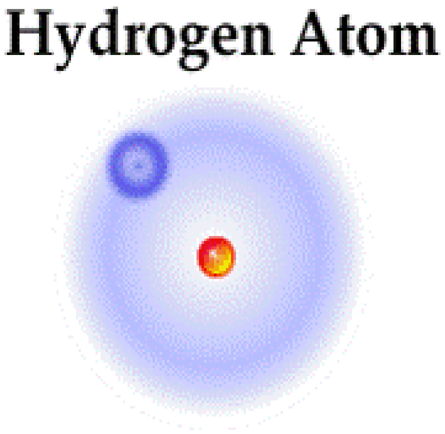
Given a Hamiltonian H for a quantum system S:

- Compute the ground energy E_0 (lowest eigenvalue of H)
- Compute some property of the ground state $|v_0\rangle$

An Example of a Quantum System and Its Hamiltonian



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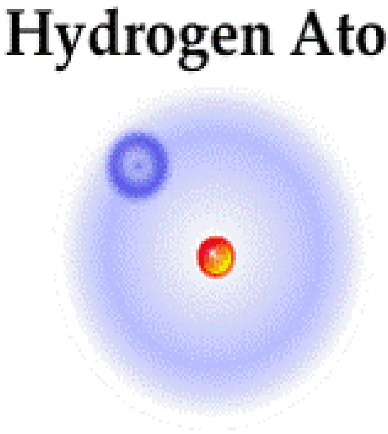

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The Hamiltonian describes the energy as a function of the electron location:

$$\hat{H} = -\frac{h^2}{2m_e}\Delta^2 - \frac{e^2}{4\pi\epsilon_0 r}$$

$$\Delta^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial}{\partial\phi^2}$$

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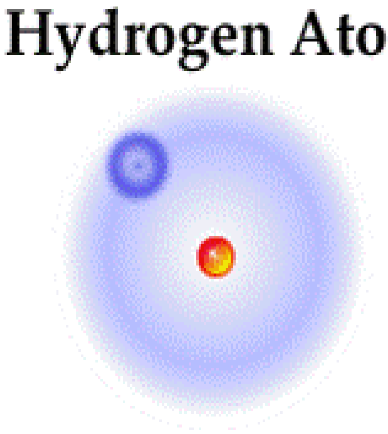

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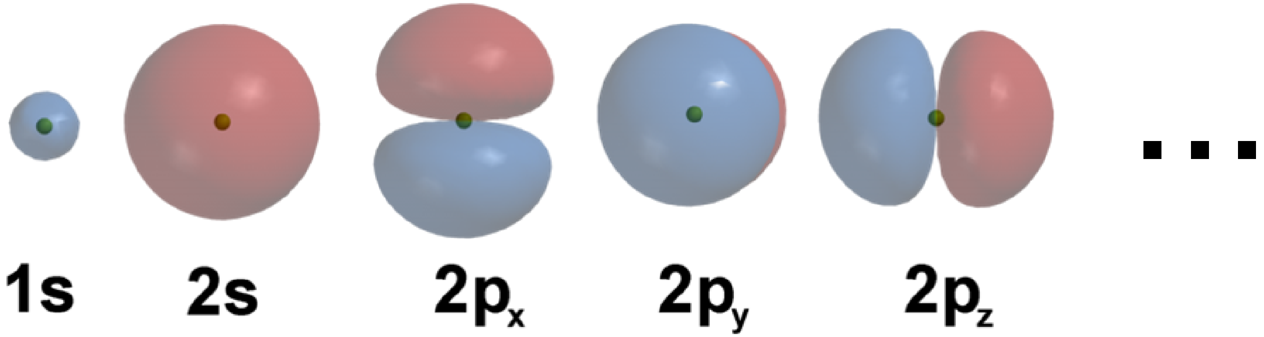
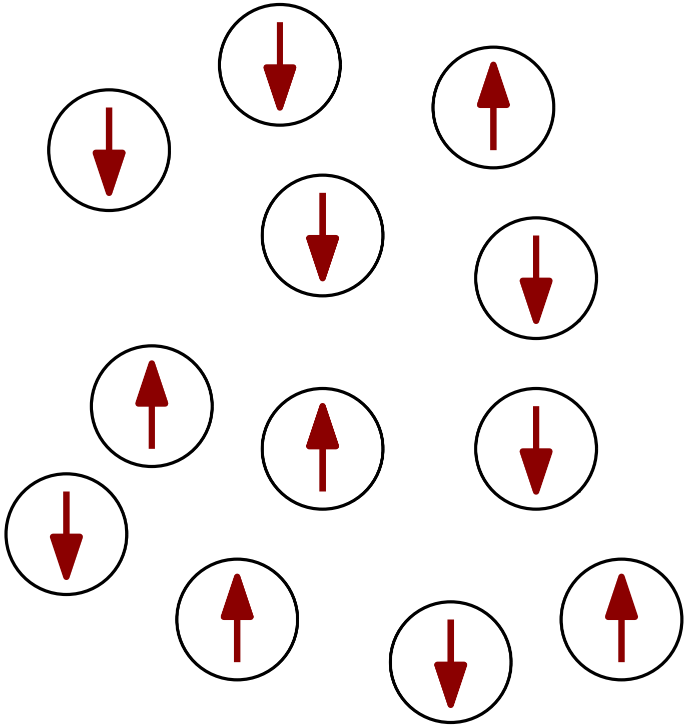


Local Hamiltonians



Quantum system composed of *n* interacting finite dimensional particles.

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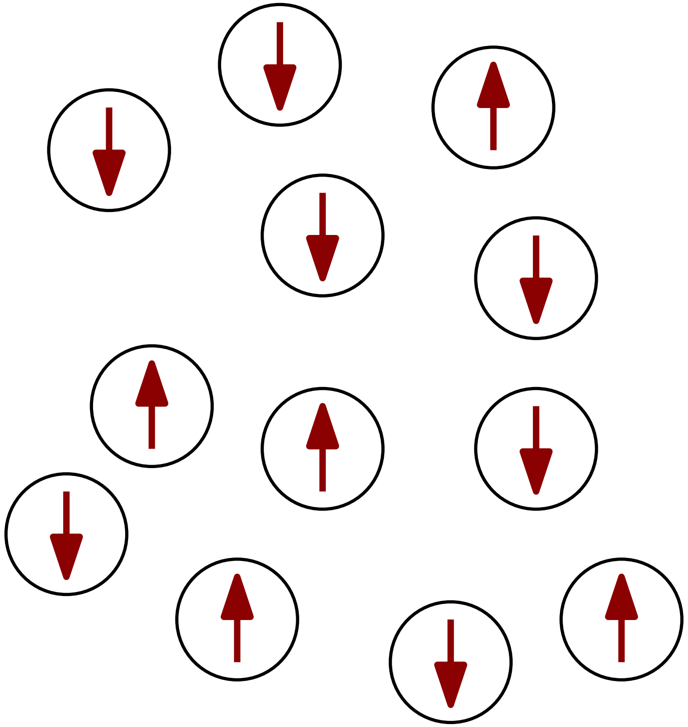

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Hilbert space for a particle: $\mathbb{C}^d$

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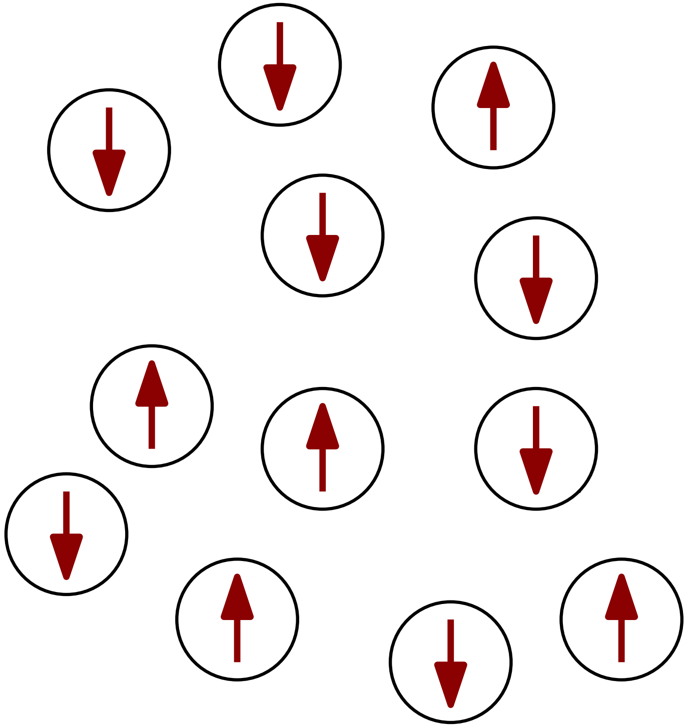

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Hilbert space for the whole system:

$$\left(\mathbb{C}^d\right)^{\otimes n}$$

Dimension = d^n

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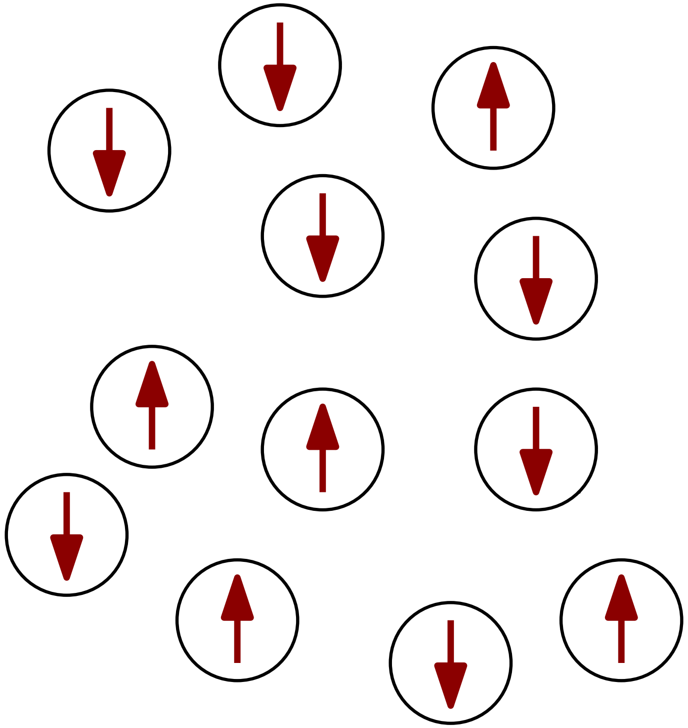

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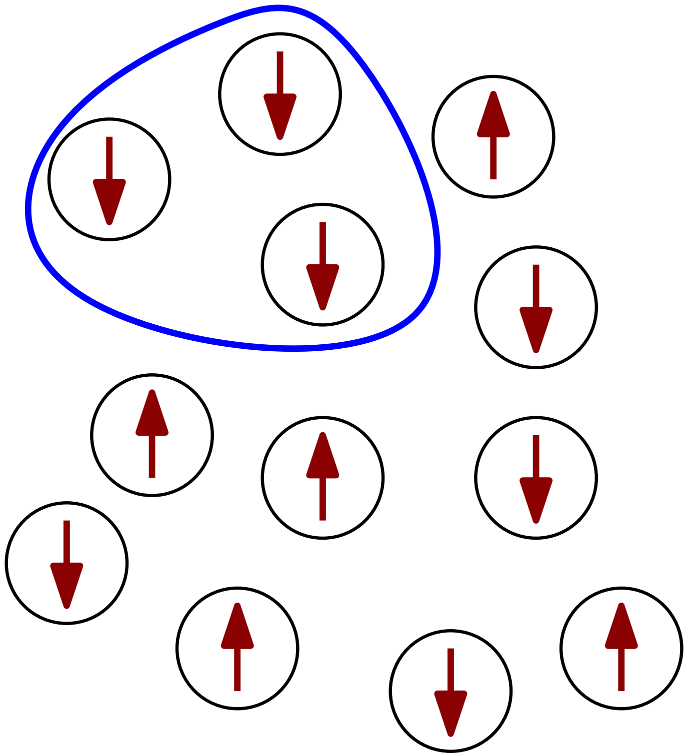

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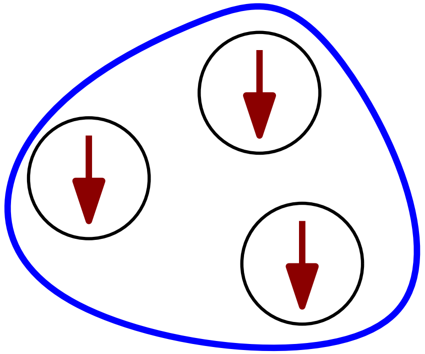

The Hamiltonian for a 3-qubit system is an 8 × 8 matrix $H_{1,2,3}$.

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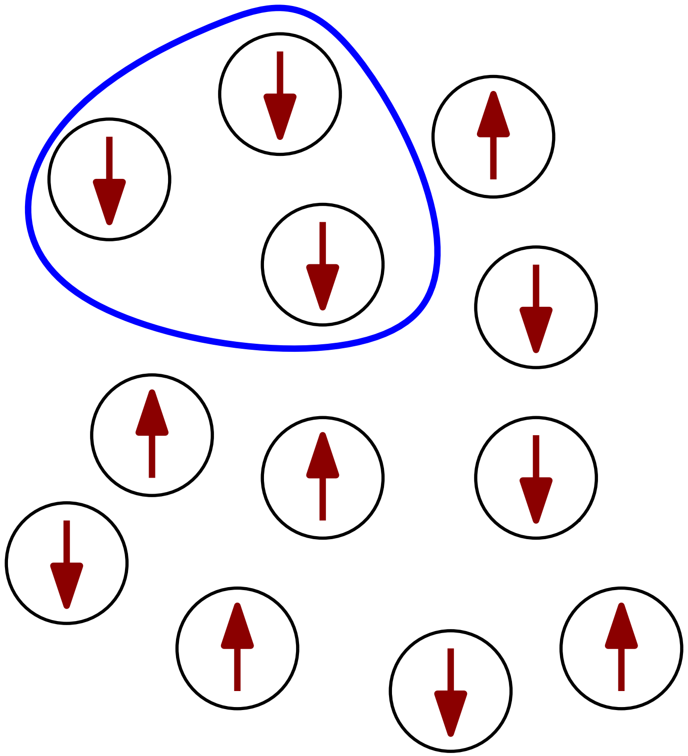

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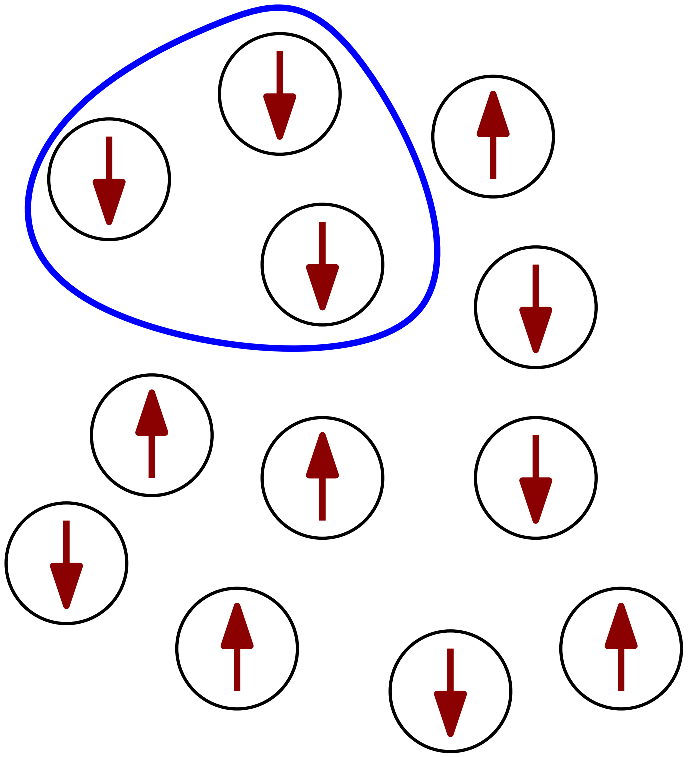
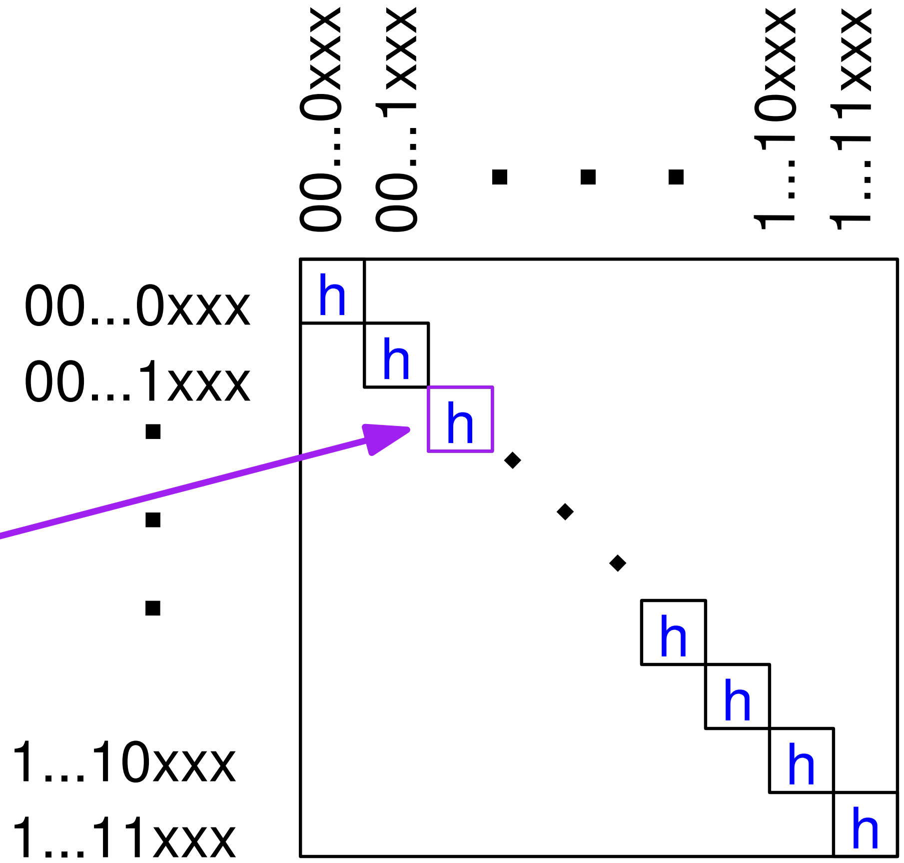


$h = H_{n-2,n-1,n}$

$I_{1,\ldots,n-3} \otimes H_{n-2,n-1,n}$



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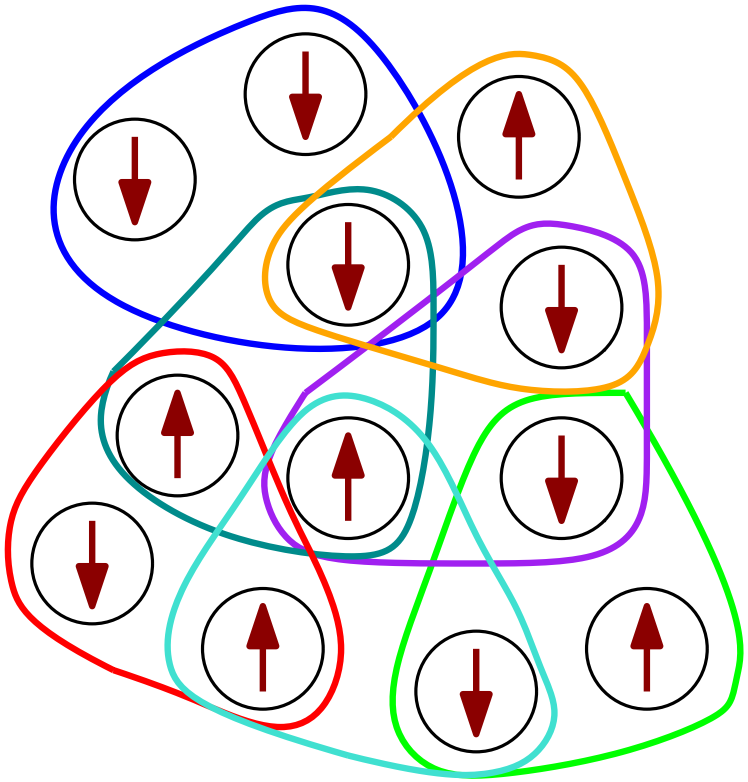

$H = \sum_a H_a$

where each H_a acts on at most k qudits

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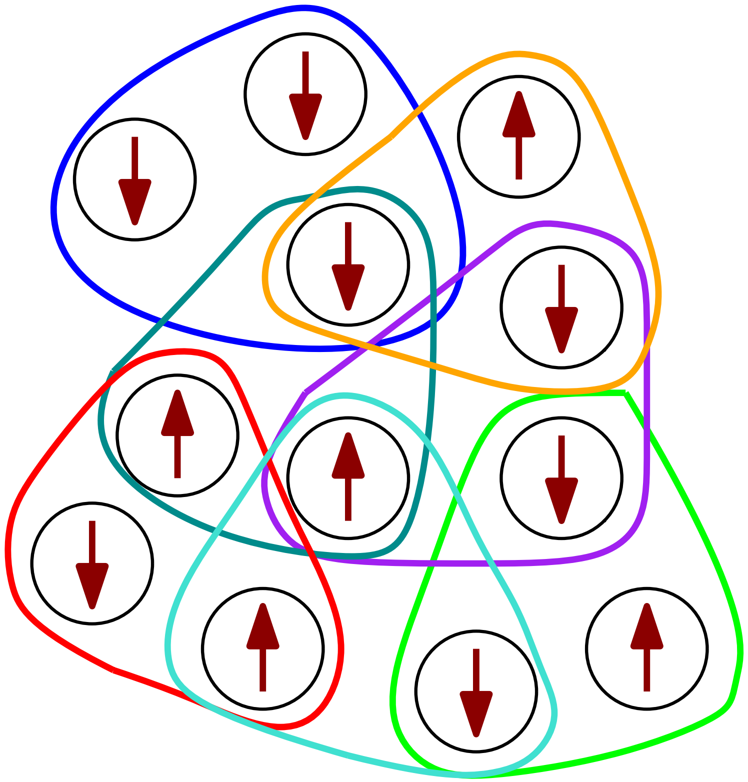

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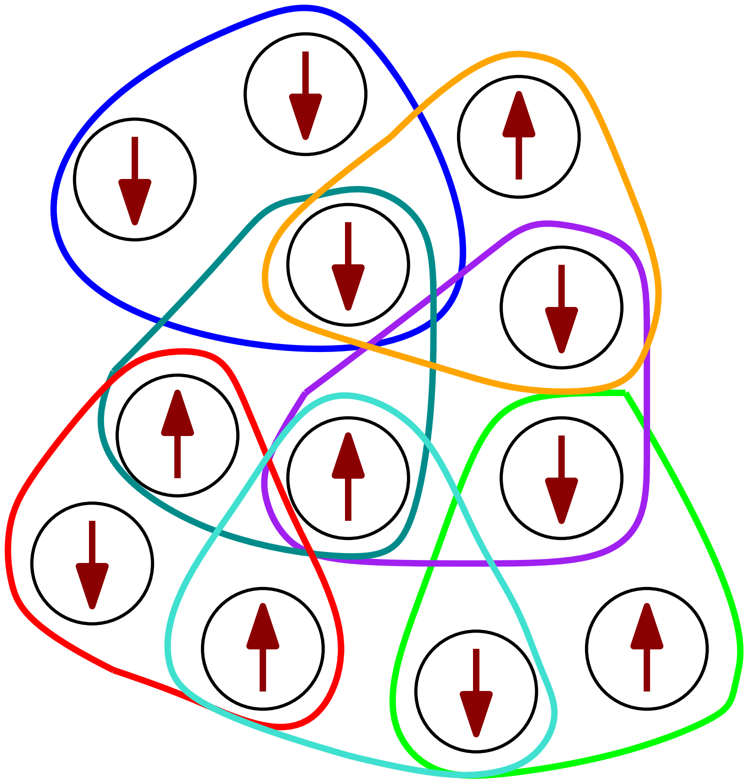

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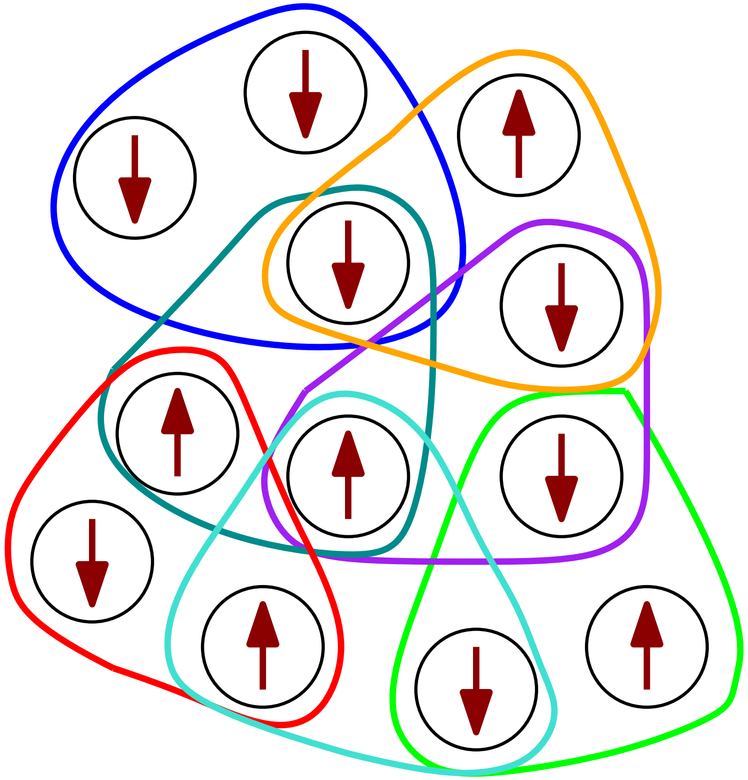

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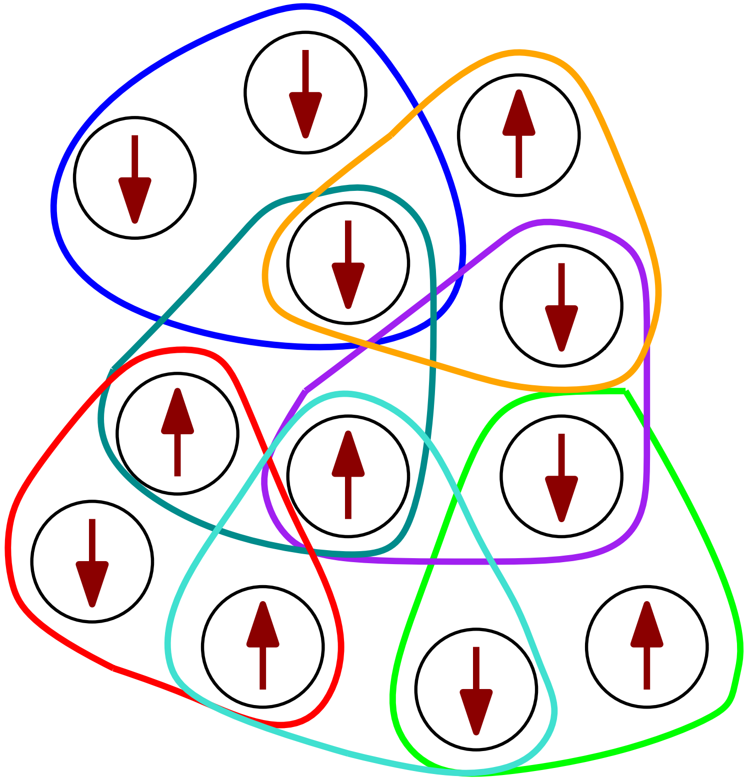

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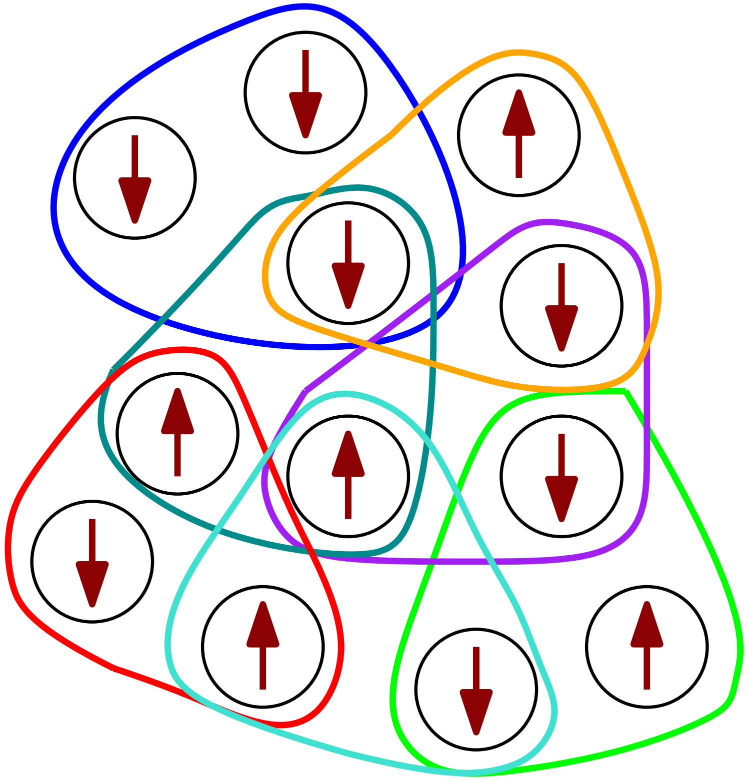
What is the ground state of the quantum system?

Local Hamiltonians



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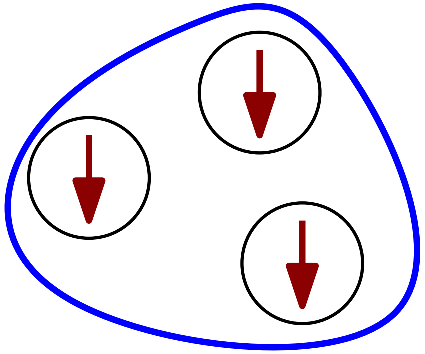
Input: Hamiltonian H, real numbers E and Δ
Is the ground energy of $H \leq E$ or $\geq E + \Delta$?

Local Hamiltonian Variations



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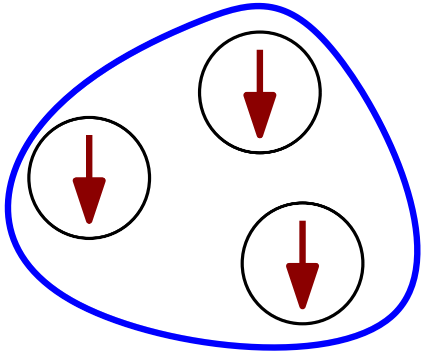

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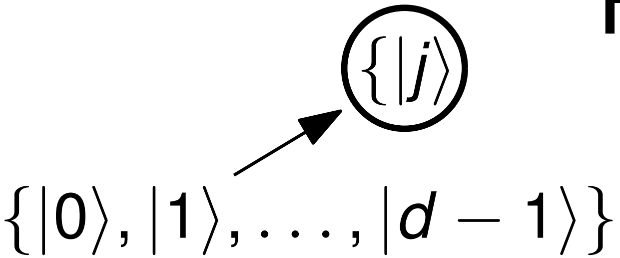

$\{|0\rangle, |1\rangle, \ldots, |d-1\rangle\}$

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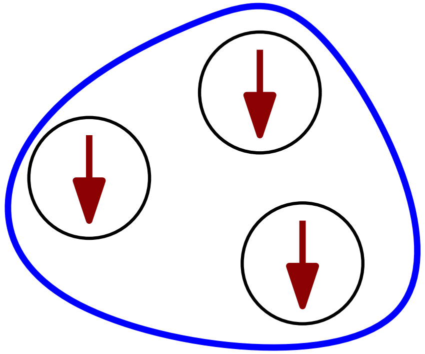

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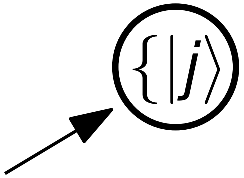

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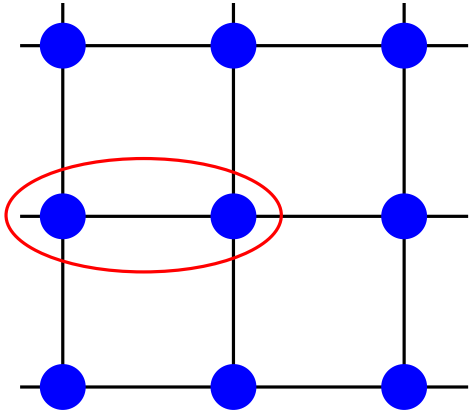
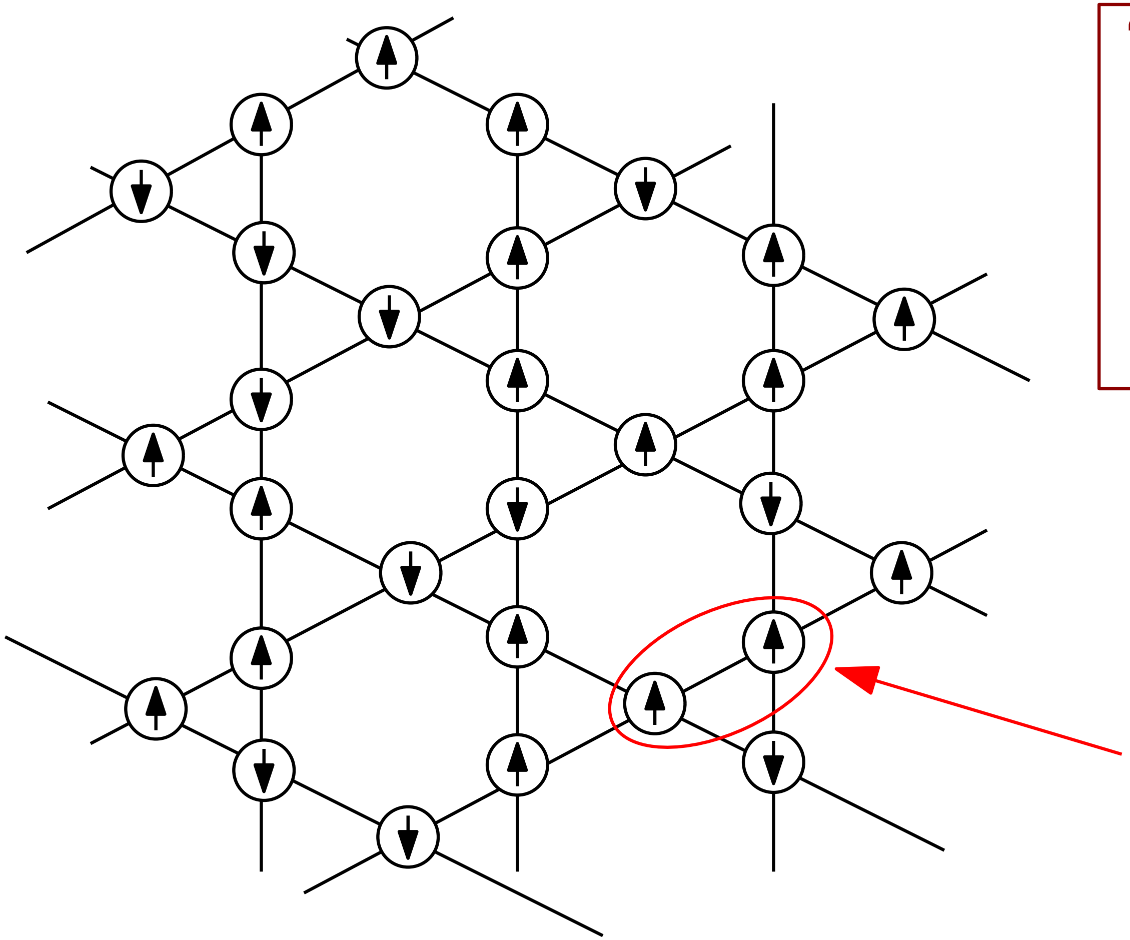
Geometry





Kagome Lattice

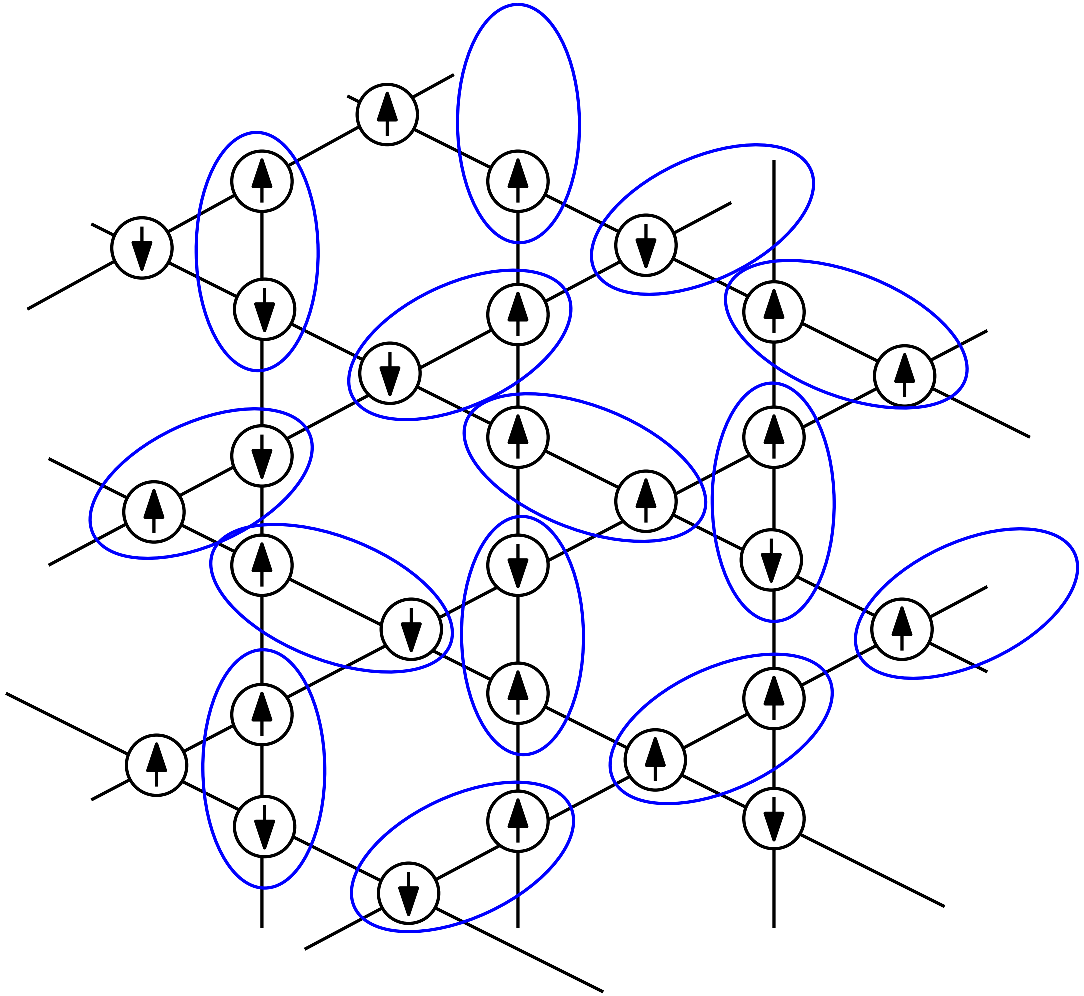
“Spin-Liquid Ground State of the $S = \frac{1}{2}$ Kagome Heisenberg Antiferromagnet”

Yan, Huse, White

Science, Vol 332, June 3, 2011

$$\begin{array}{c|cccc} & \mathbf{00} & \mathbf{01} & \mathbf{10} & \mathbf{11} \\ \hline \mathbf{00} & 1 & 0 & 0 & 0 \\ \mathbf{01} & 0 & -1 & -2 & 0 \\ \mathbf{10} & 0 & -2 & -1 & 0 \\ \mathbf{11} & 0 & 0 & 0 & 1 \end{array}$$

Heisenberg
- Antiferromagnet
Model



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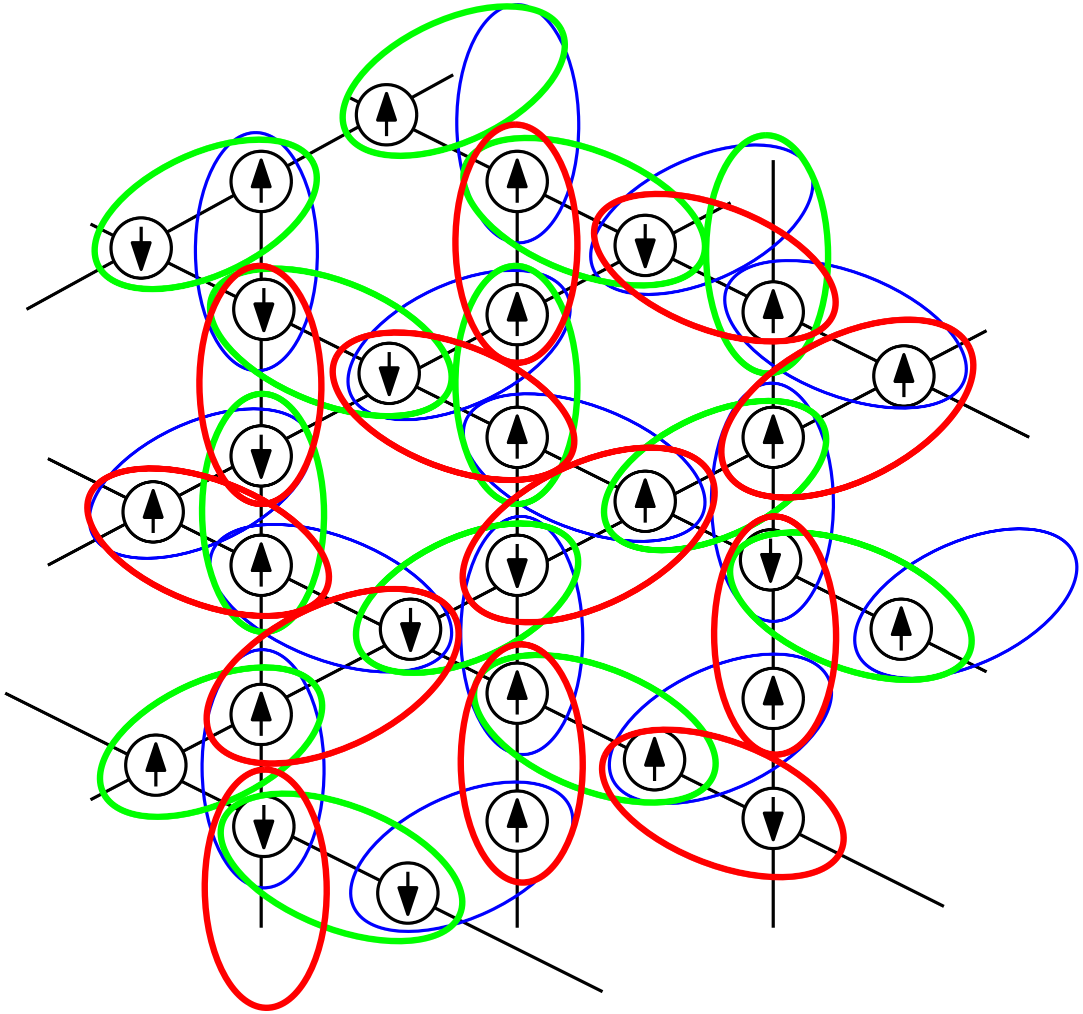

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Is the Ground State a Valence Bond Crystal?

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What is the complexity of the Local Hamiltonian problem?

- Set of local constraints
- Find a global state that minimizes cost

”Classical” Local Hamiltonian

n d-dimensional particles: $\mathcal{H} = \left(\mathbb{C}^d\right)^{\otimes n}$

Standard basis denoted by classical strings: $\left|x_1, x_2, \ldots, x_n\right\rangle$

Each $x_i \in \left\{0, \ldots, d-1\right\}$

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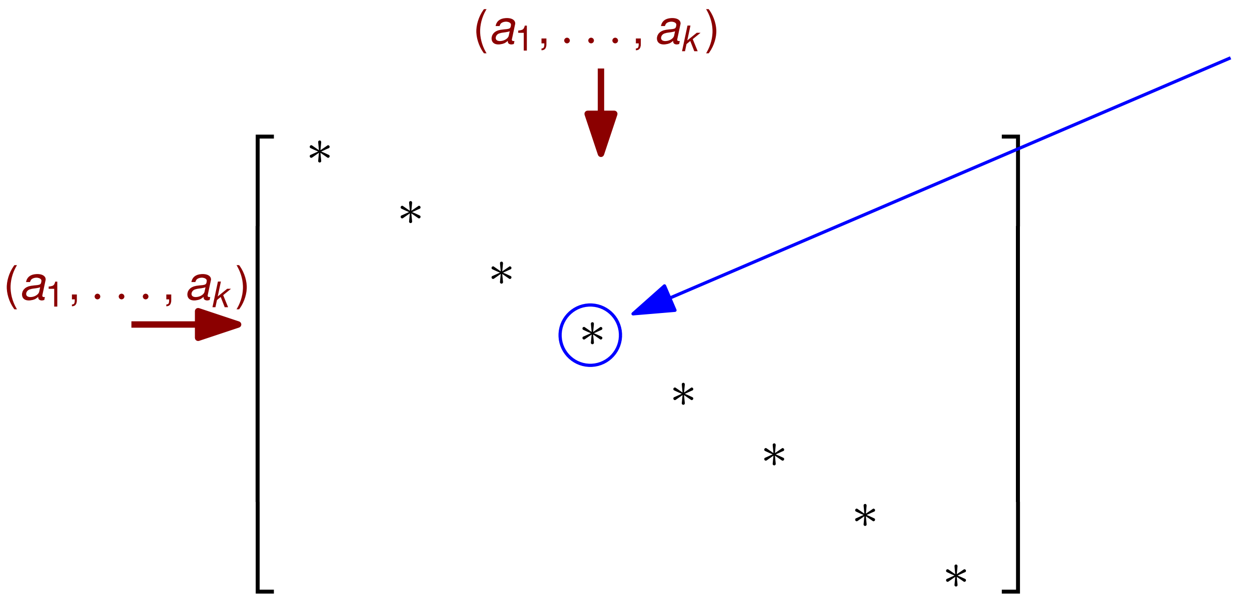
H_j operates on particles $i_1, i_2, \ldots, i_k$



Cost/Energy of setting:
$x_{i_1} = a_1, \ldots, x_{i_k} = a_k$

”Classical” Local Hamiltonian

n d-dimensional particles: $\mathcal{H} = \left(\mathbb{C}^d\right)^{\otimes n}$

Standard basis denoted by classical strings: $|x_1, x_2, \ldots, x_n\rangle$

Each $x_i \in \{0, \ldots, d-1\}$

Special case of LH: $H = \sum_j H_j$

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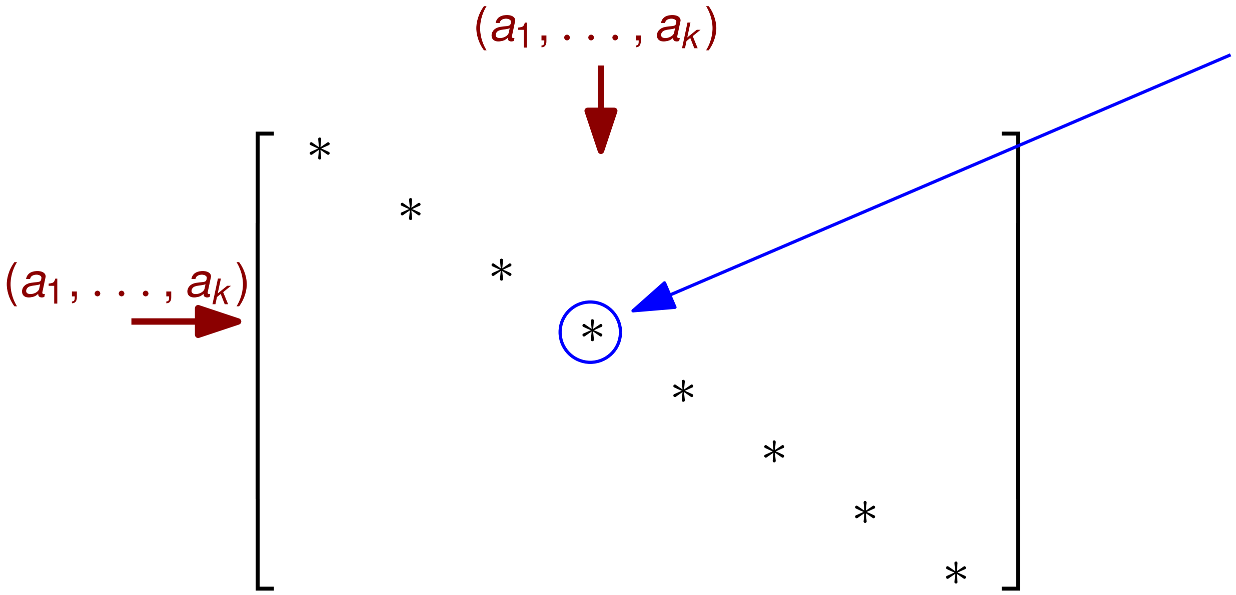

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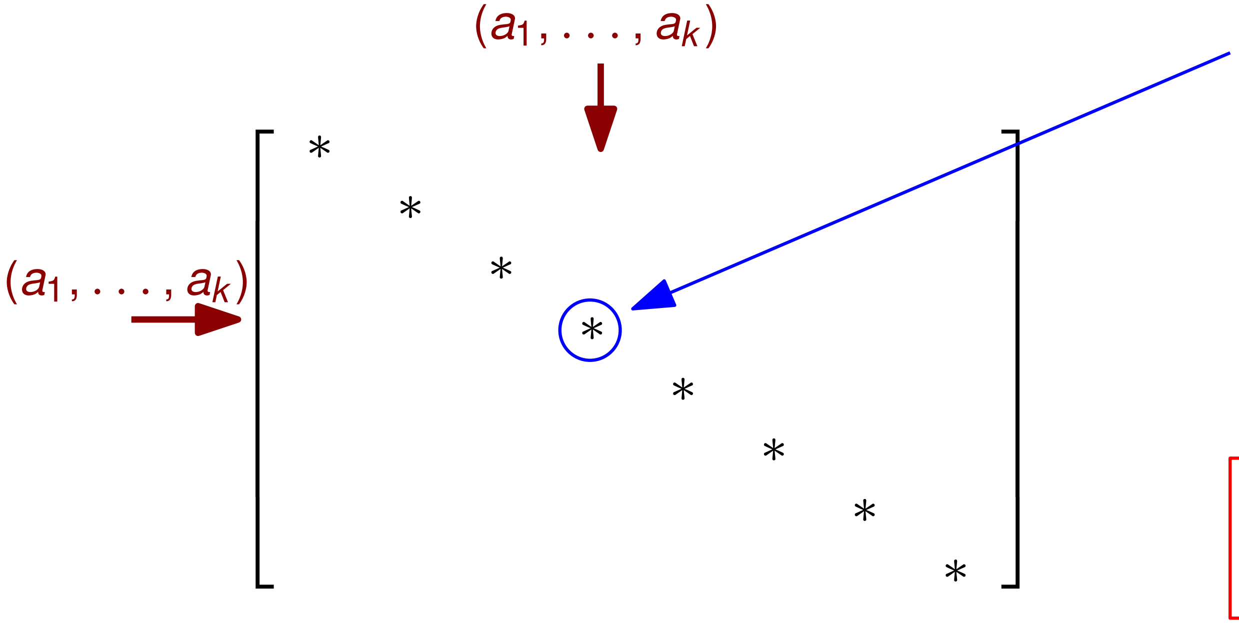

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Weighted Constraint Satisfaction Problem

Boolean Satisfiability and 3-SAT

Input: n Boolean variables $x_1, \ldots, x_n$

m clauses: $C_1, \ldots, C_m$.

C_i: disjunction of three literals. e.g., $(x_{i1} \vee \neg x_{i2} \vee x_{i3})$

Question: Is there a Boolean assignment to $x_1, \ldots, x_n$ such that

$$C_1 \wedge C_2 \wedge \cdots \wedge C_m = 1\ ?$$

Local Hamiltonian is NP-hard

$\text{3SAT} \propto \text{LH}$

Local Hamiltonian is NP-hard

$$\begin{array}{c|cccccccc}
 & & & 010 \downarrow & & & & & \\
\hline
 & 0 & & & & & & & \\
 & & 0 & & & & & & \\
010 \rightarrow & & & 1 & & & & & \\
 & & & & 0 & & & & \\
 & & & & & 0 & & & \\
 & & & & & & 0 & & \\
 & & & & & & & 0 & \\
 & & & & & & & & 0
\end{array}$$

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$$|010\rangle\langle 010| = \begin{array}{r c} & \begin{array}{cccccccc} & & 010 & & & & & \\ & & \downarrow & & & & & \end{array} \\ 010 \rightarrow & \begin{bmatrix} 0 & & & & & & & \\ & 0 & & & & & & \\ & & 1 & & & & & \\ & & & 0 & & & & \\ & & & & 0 & & & \\ & & & & & 0 & & \\ & & & & & & 0 & \\ & & & & & & & 0 \end{bmatrix} \end{array} \Leftrightarrow (x \vee \neg y \vee z)$$

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$3SAT \propto LH$

$$H = \sum_j H_{C_j} \quad \Leftrightarrow \quad C_1 \wedge C_2 \wedge \cdots \wedge C_m$$

H has a zero energy ground state $\Leftrightarrow$ $C_1 \wedge C_2 \wedge \cdots \wedge C_m$ is satisfiable.

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$\text{SAT} \in \text{NP}$

x encodes an instance of 3-SAT

Witness y:
satisfying assignment $y_i = 0/1$

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Poly-sized circuit family $\{C_n\}$

If $|x| = n$, then

$A(x, y)$ accepts $\leftrightarrow C_n(x, y) = 1$

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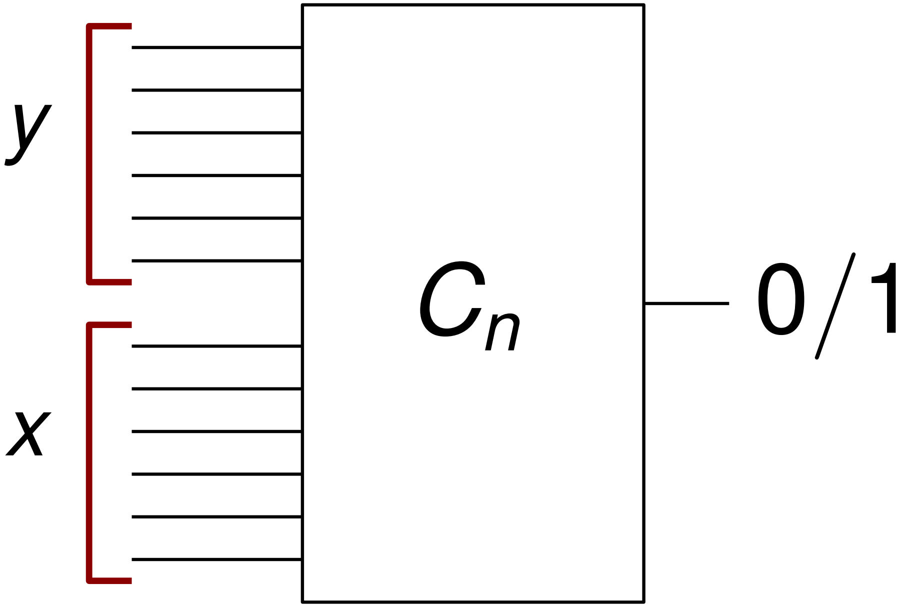

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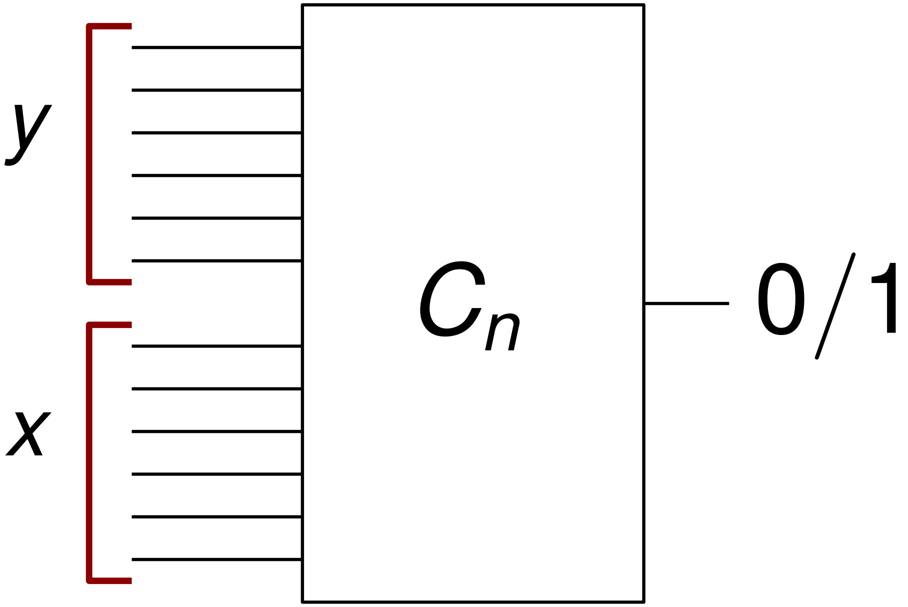

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The circuit family $\{C_n\}$ must be *uniform*:
There is a polynomial time Turing Machine that computes C_n on input 1^n

Promise Problems

Decision Problems: answer is ”Yes” or ”No”

$L \subseteq \{0, 1\}^*$

$x \in L \Rightarrow$ ”Yes”

$x \notin L \Rightarrow$ ”No”

Promise Problems: input strings partitioned into 3 sets

$$\text{Yes} \cup \text{No} \cup \text{Invalid} = \{0, 1\}^*$$

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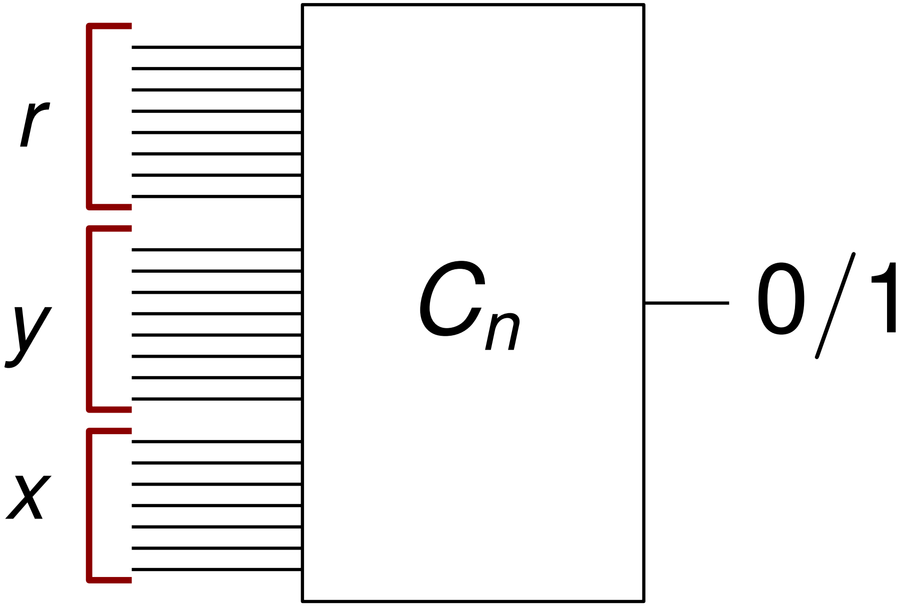
Uniform, polynomial-sized circuit family $\{C_n\}$: iff $|x| = n$, then

$x \in \text{Yes} \leftrightarrow \exists y$ such that
$\text{Prob}_r[C_n(x, y, r) = 1] \geq \frac{2}{3}$

$x \in \text{No} \leftrightarrow \forall y$
$\text{Prob}_r[C_n(x, y, r) = 1] \geq \frac{1}{3}$



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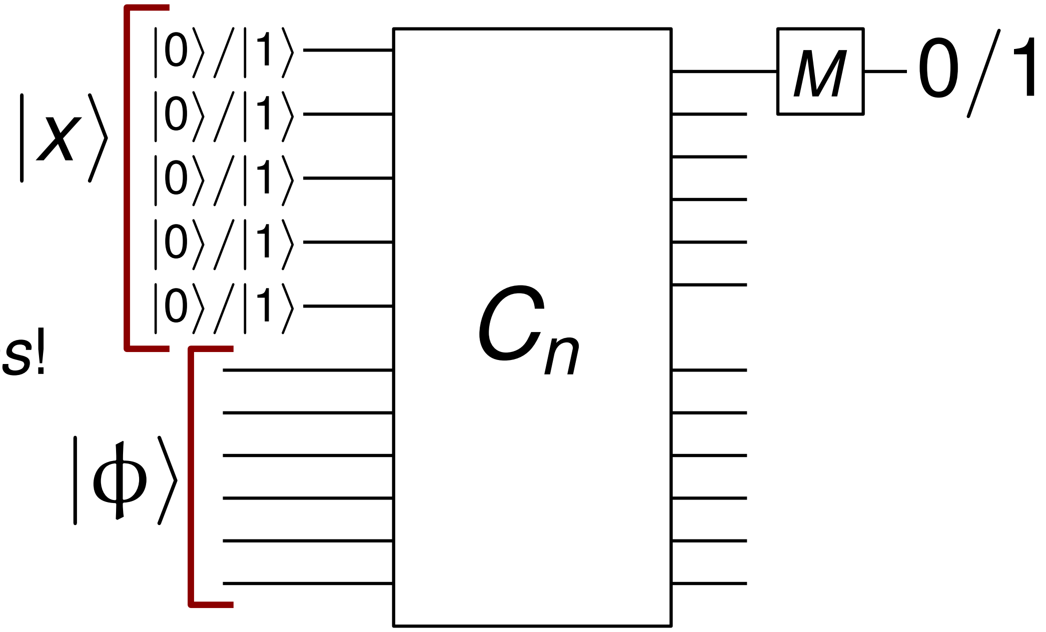

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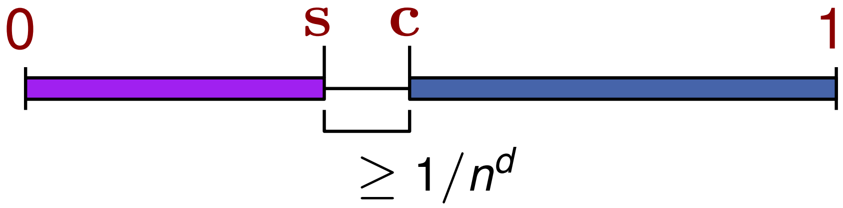

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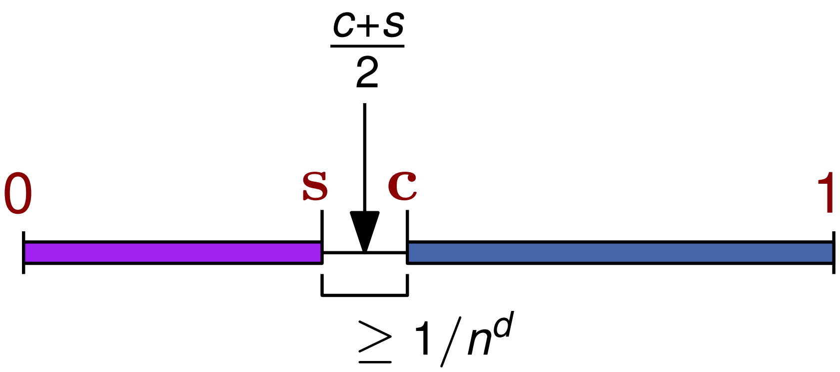

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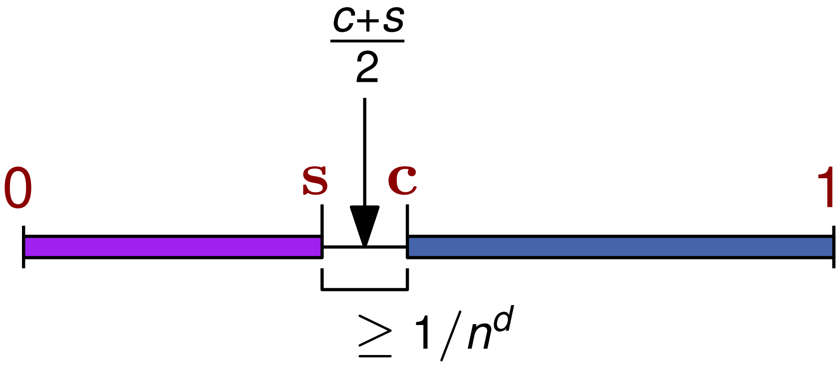

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By Chernoff's Inequality
For m = sufficiently large polynomial in n,
Probability number of accepts deviates from the expectation by more than $\left(\frac{c-s}{2}\right) m$ is exponentially small

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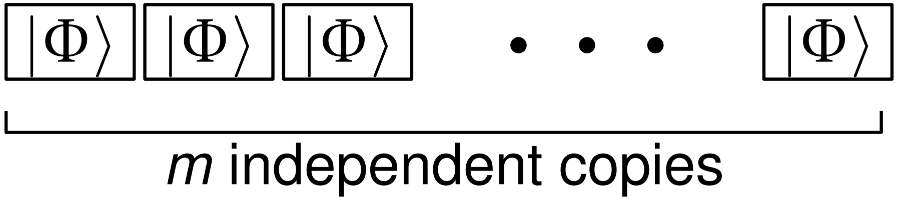

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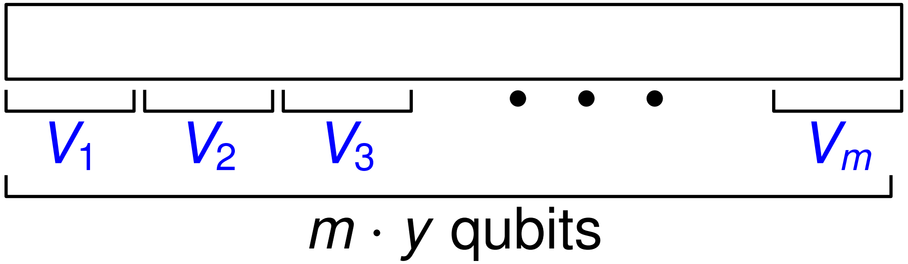

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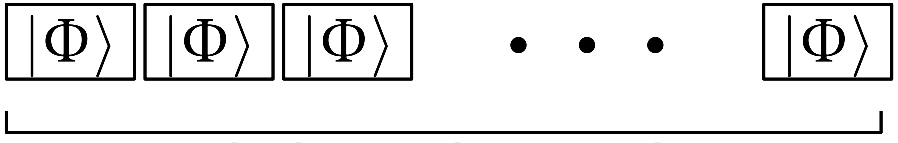

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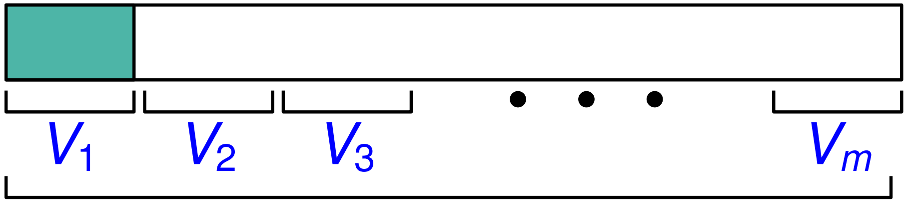

$m \cdot y$ qubits

Prob ACC $\leq s$

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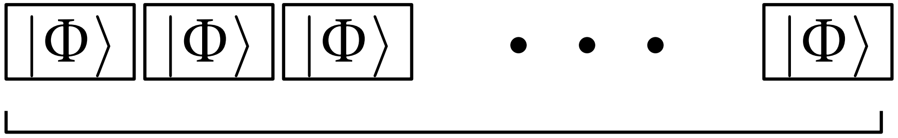

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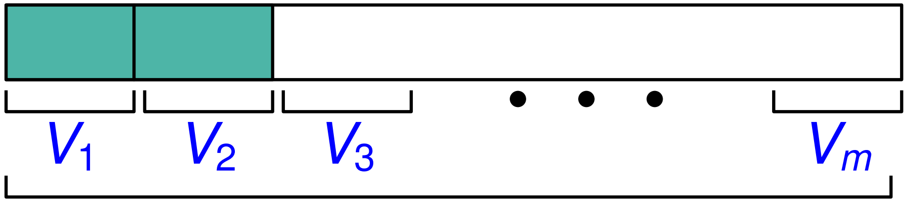

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Even when conditioned on outcome of V_1's measurement

The class QMA - amplification

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A *promise* problem is in QMA if there is a poly-sized uniform **quantum** circuit family $\{C_n\}$ such that on input x, where $|x| = n$:

If $\underline{x \in \text{Yes}}$, then there is a **quantum** witness $|\phi\rangle$ such that $\text{Prob}[C_n(x, |\phi\rangle) = 1] \geq \mathbf{c}$

If $\underline{x \in \text{No}}$, then for every $|\phi\rangle$, $\text{Prob}[C_n(x, |\phi\rangle) = 1] \leq \mathbf{s}$

$|\phi\rangle$ has $y = \text{poly}(n)$ qubits.

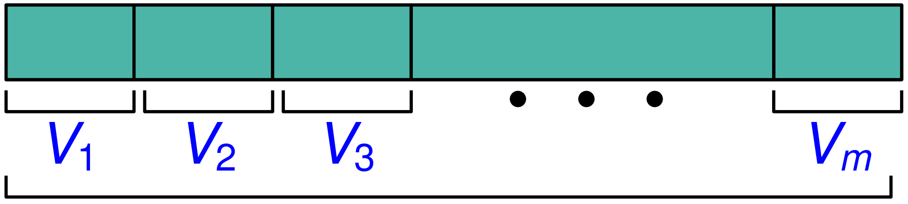
If $c - s \geq \frac{1}{n^d}$, then

$$\text{QMA}(c, s) = \text{QMA}\left(1 - \frac{1}{2^n}, \frac{1}{2^n}\right)$$

Completeness:

$$\underbrace{\boxed{|\Phi\rangle}\boxed{|\Phi\rangle}\boxed{|\Phi\rangle}\quad \cdots \quad \boxed{|\Phi\rangle}}_{m \text{ independent copies}}$$

Soundness:



$m \cdot y$ qubits

Prob ACC $\leq s$

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Even when conditioned on outcome of V_1's measurement

The Marriott-Watrous "Trick"

QMA$_y$(c, s)

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for every polynomial y

Probabilistically try and back up after a measurement.

Measure for a successful back up.

Principle of deferred measurements.

Complexity Classes and Complete Problems

NP $\subseteq$ MA $\subseteq$ QMA

Complexity Classes and Complete Problems

$$\mathrm{NP} \subseteq \mathrm{MA} \subseteq \mathrm{QMA} \subseteq \mathrm{PP} \subseteq \mathrm{PSPACE}$$

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Boolean satisfiability
is complete for NP
[Cook-Levin]

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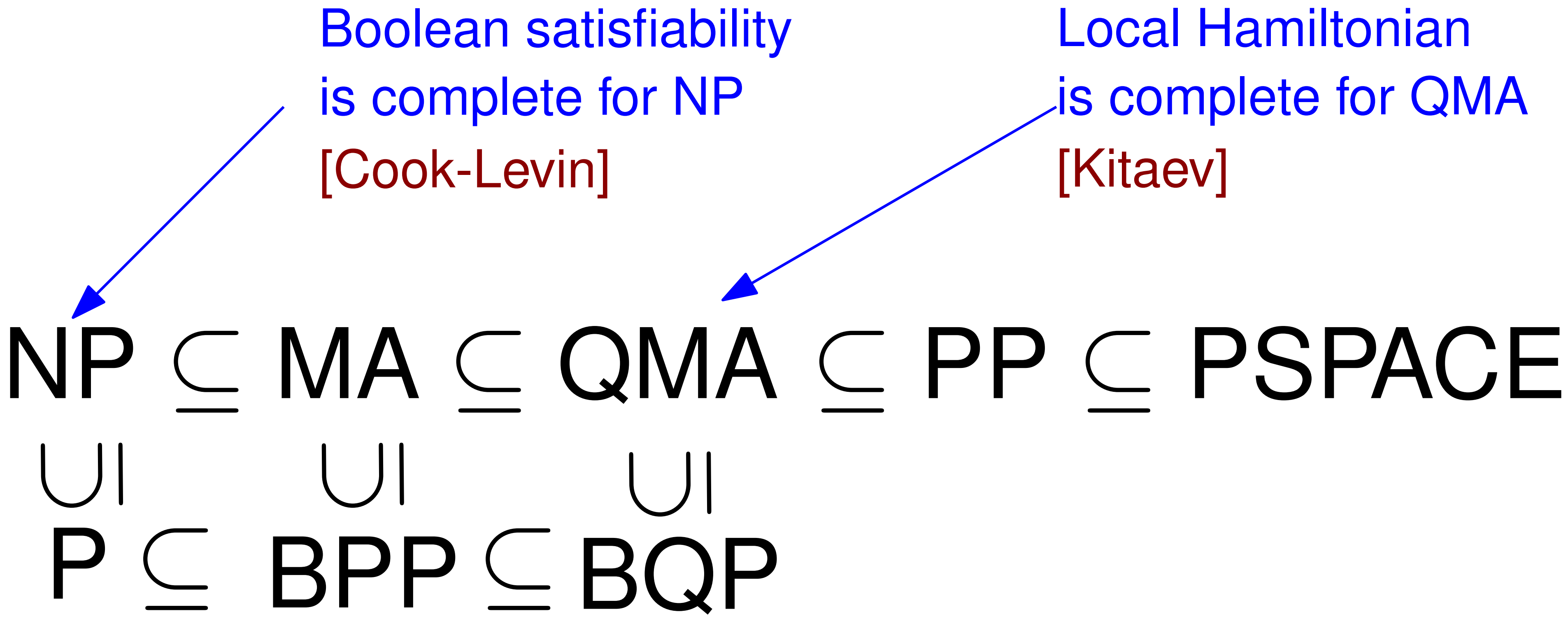

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$$\begin{tikzcd}
\mathrm{NP} \arrow[r, phantom, "\subseteq"] & \mathrm{MA} \arrow[r, phantom, "\subseteq"] & \mathrm{QMA} \arrow[r, phantom, "\subseteq"] & \mathrm{PP} \arrow[r, phantom, "\subseteq"] & \mathrm{PSPACE} \\
\mathrm{P} \arrow[u, phantom, "\rotatebox{90}{$\subseteq$}"] \arrow[r, phantom, "\subseteq"] & \mathrm{BPP} \arrow[u, phantom, "\rotatebox{90}{$\subseteq$}"] \arrow[r, phantom, "\subseteq"] & \mathrm{BQP} \arrow[u, phantom, "\rotatebox{90}{$\subseteq$}"] & &
\end{tikzcd}$$

The Local Hamiltonian Problem

Input:

$H_1, \ldots, H_r$, set of Hermitian positive semi-definite matrices operating on k qudits of dimension d, with bounded norm $\|H_i\| \leq 1$.

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or are all eigenvalues $\geq E + \Delta$?

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Eigenvalues of each H_i in $[0, 1]$.

$H_i + \alpha I \rightarrow$ eigenvalues of H shift by α

$\alpha H \rightarrow$ eigenvalues of H scale by factor of α

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Local Hamiltonian is in QMA

Boolean
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Is $\Phi(y)$ satisfiable?

Witness: Satisfying assignment *y*

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$\Longrightarrow$

Need a measurement whose outcome = 1 with probability $\propto \langle \Phi | H | \Phi \rangle$.

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Add auxiliary bit and implement unitary:

For every j:

$$|v_{aj}\rangle|0\rangle \quad \Rightarrow \quad |v_{aj}\rangle \left(\sqrt{1-\lambda_{aj}}|0\rangle + \sqrt{\lambda_{aj}}|1\rangle \right)$$

Measure last qubit

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$$|\Phi\rangle|0\rangle = \sum_j \alpha_{aj} \underbrace{|v_{aj}\rangle}_{k \text{ qubits } H_a \text{ acts on}} \underbrace{|\beta_{aj}\rangle}_{\text{the rest of the qubits}} |0\rangle$$

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Probability of measuring 1 (overall):

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either $\leq E/r$ OR $\geq (E + \Delta)/r$

Boolean Satisfiability is NP-hard [Cook-Levin]

Start with a generic language L in NP

Is $x \in L$?

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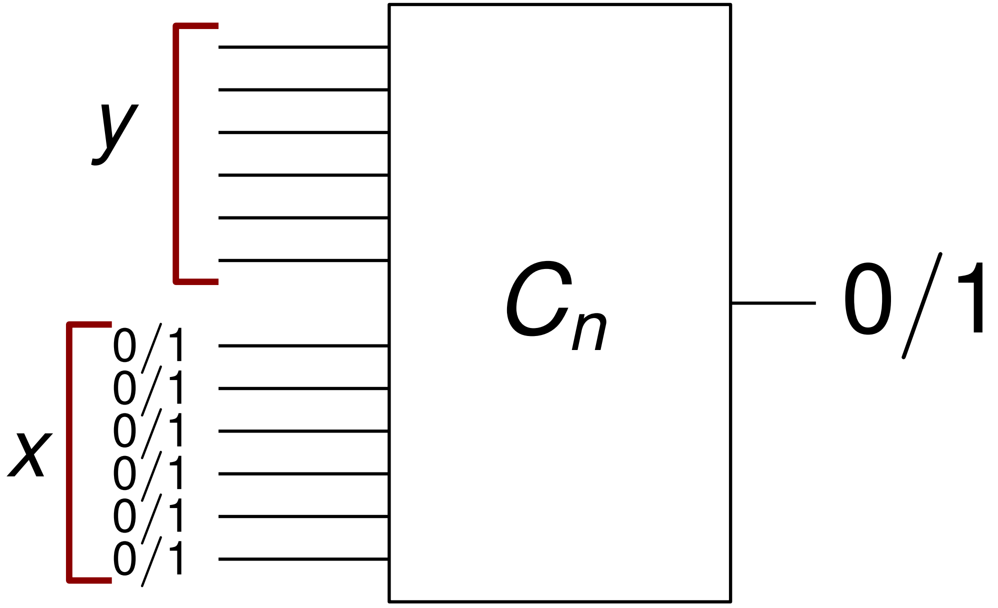

Is there a string y that causes this circuit to output 1?

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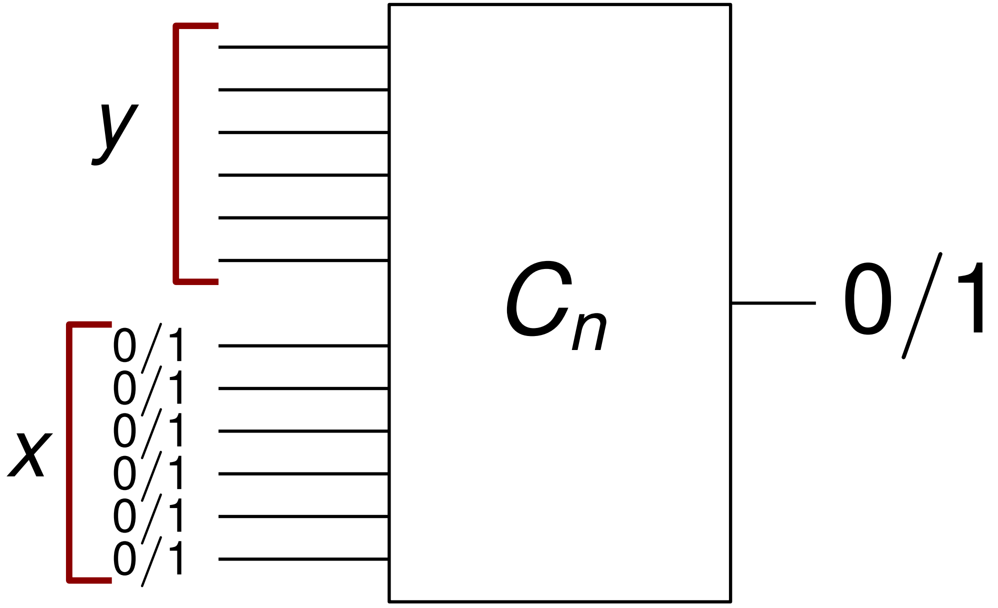

$\Rightarrow$

Boolean
Formula:
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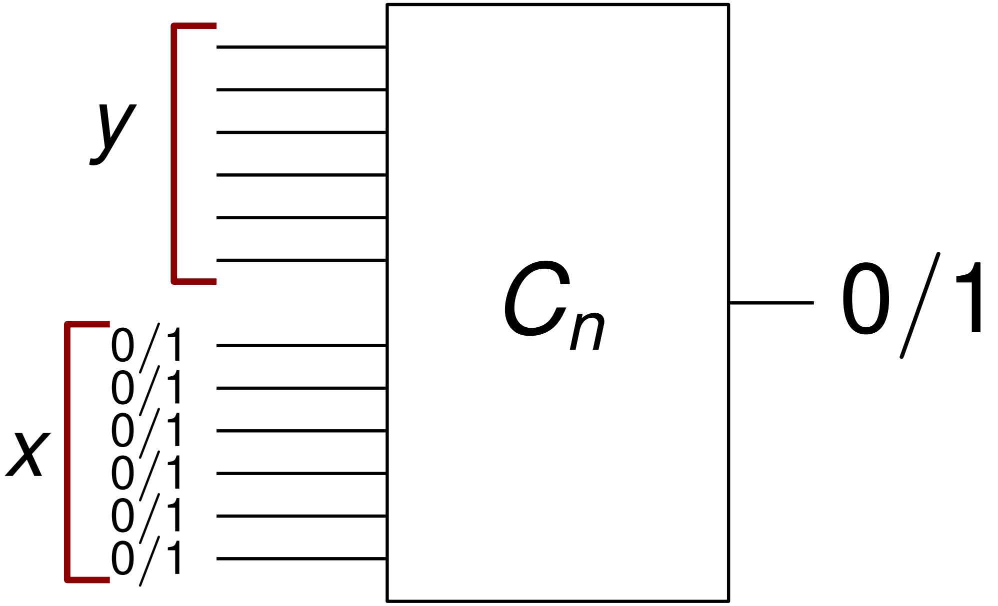

$\Rightarrow$

Boolean Formula: $\Phi_x(y)$

Is there a string y that causes this circuit to output 1? $\Leftrightarrow$ Is $\Phi_x(y)$ satisfiable?

Local Hamiltonian is QMA-hard

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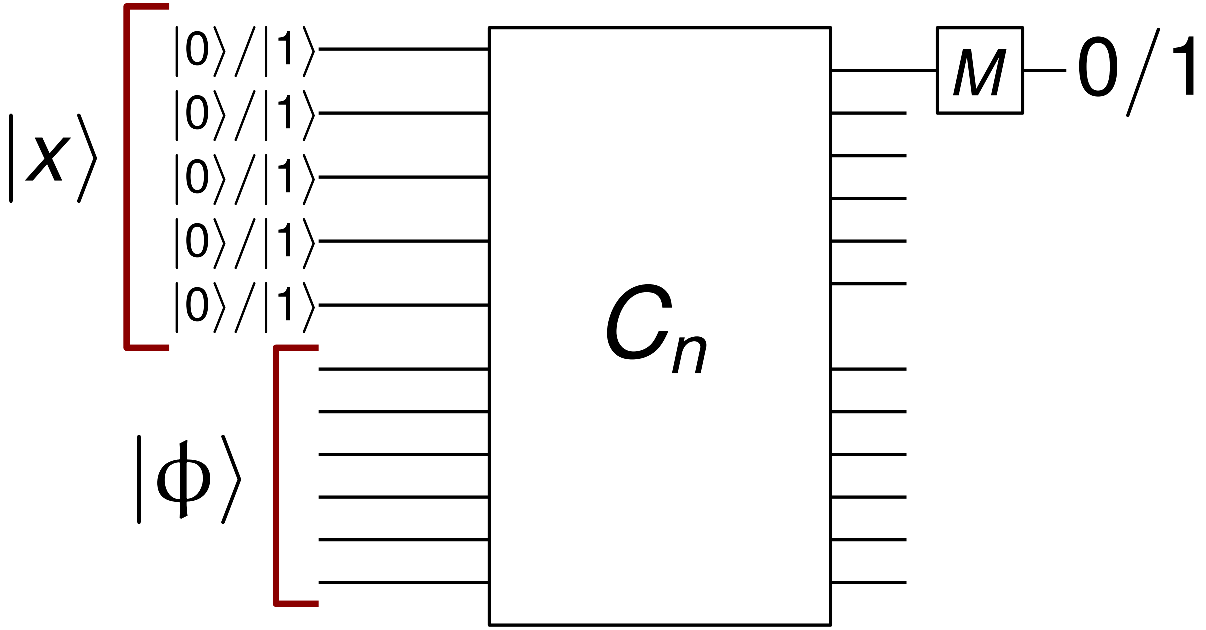

Is there a quantum state $\phi\rangle$
that causes this quantum circuit
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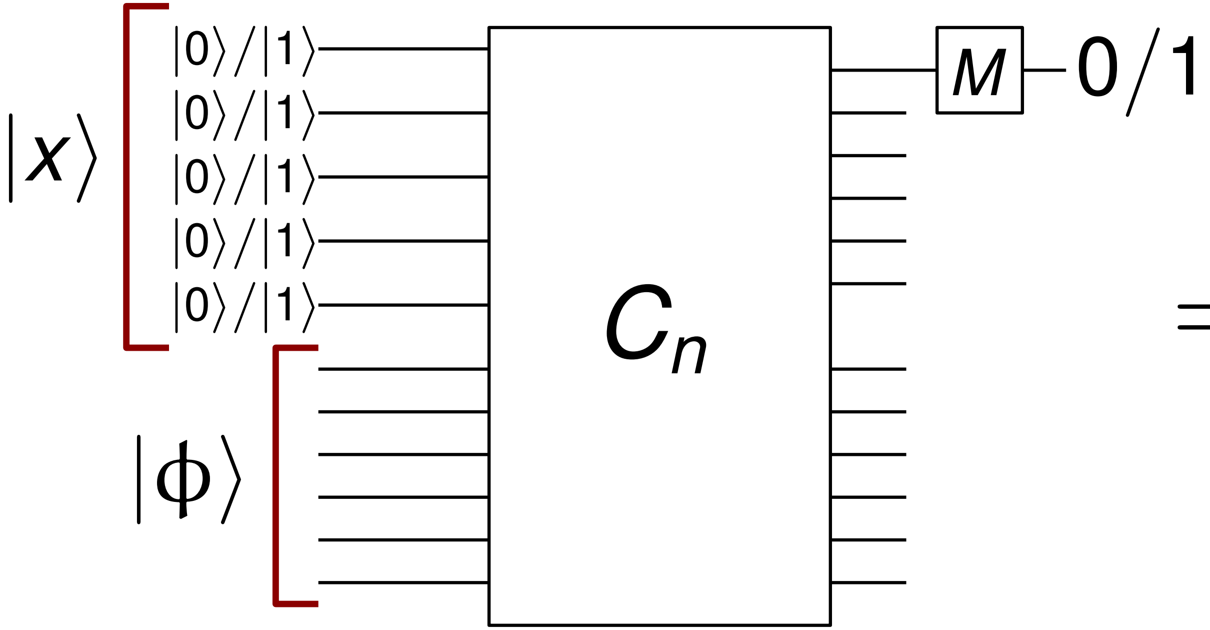

$\Rightarrow$ 5-Local Hamiltonian: (H_x, E, Δ)

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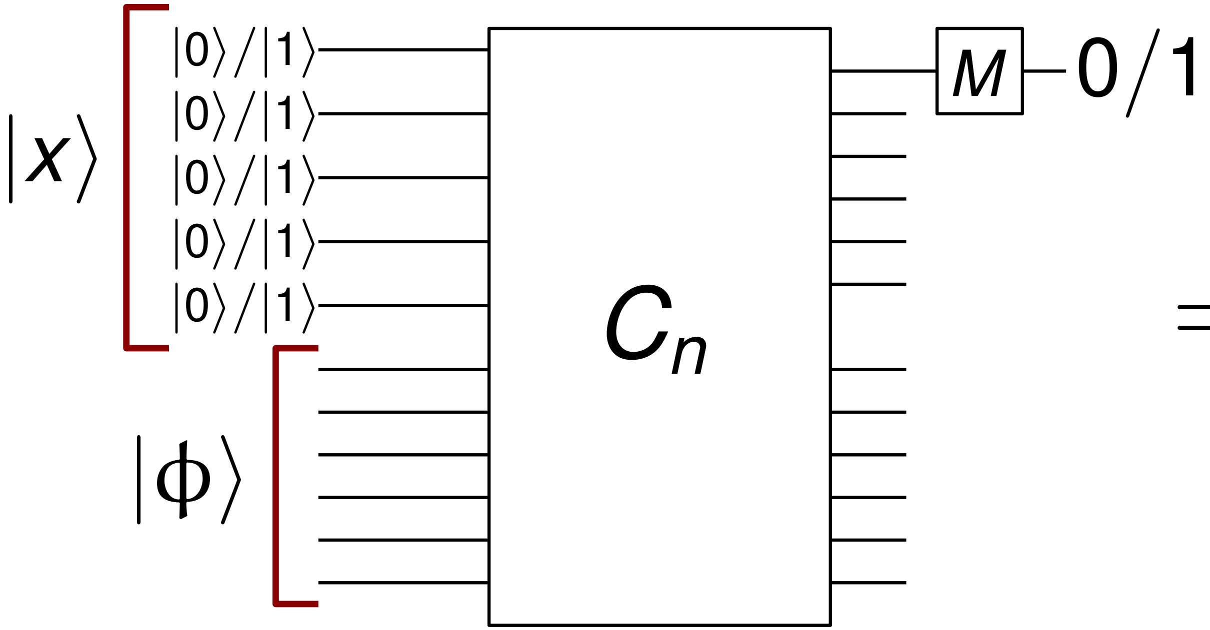

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$\Rightarrow$ Ground energy of $H_x \leq E$

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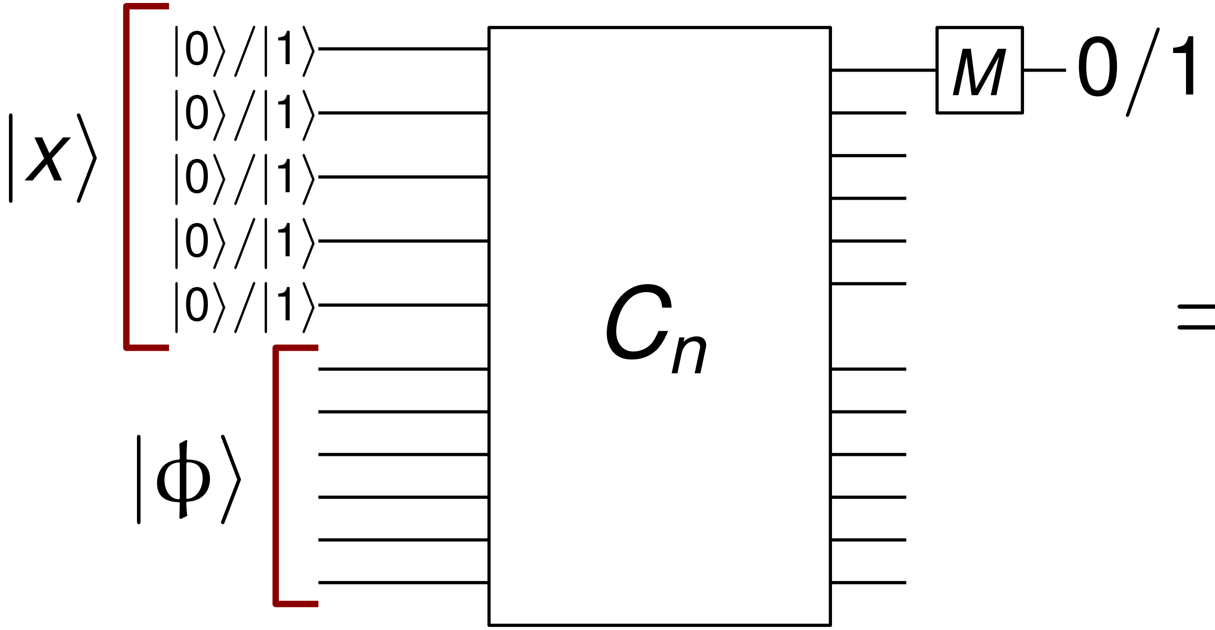

$\Rightarrow$ 5-Local Hamiltonian: (H_x, E, Δ)

Is there a quantum state $\phi\rangle$ that causes this quantum circuit to output 1 with high probability? $\Rightarrow$ Ground energy of $H_x \leq E$

For every $|\phi\rangle$, circuit outputs 0 w.h.p. $\Rightarrow$ Ground energy of $H_x \geq E + \Delta$

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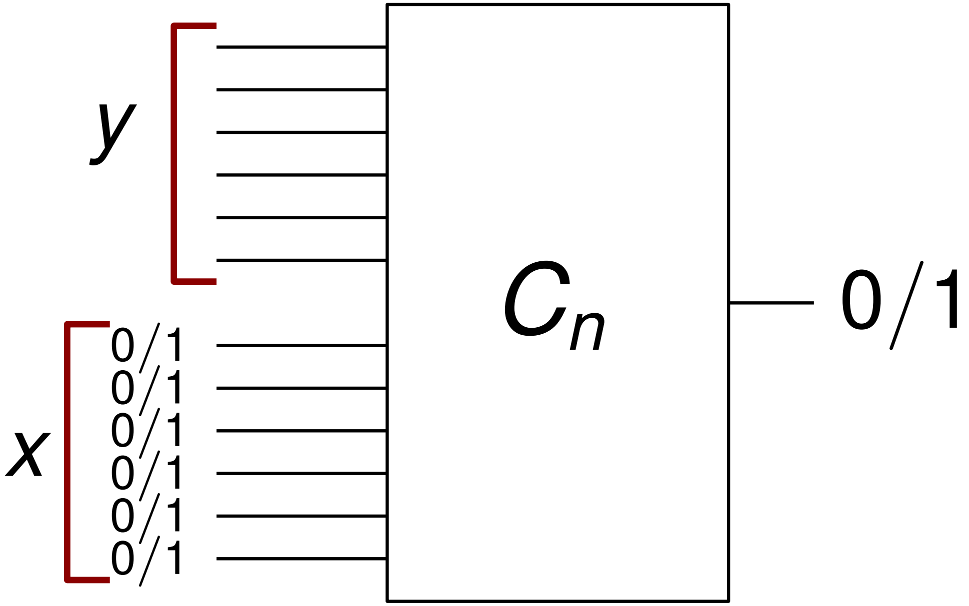

Is there a string y that causes this circuit to output 1?

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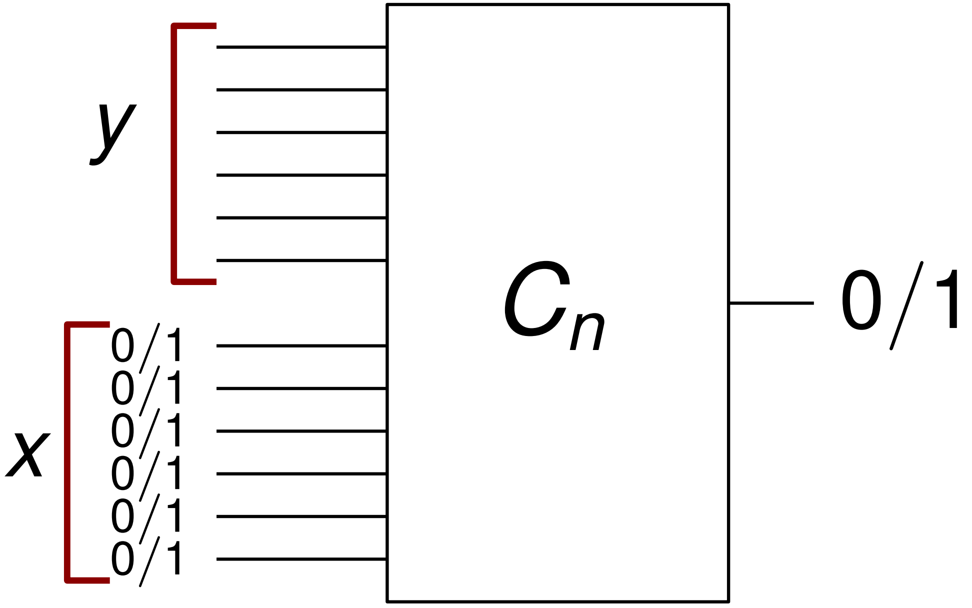

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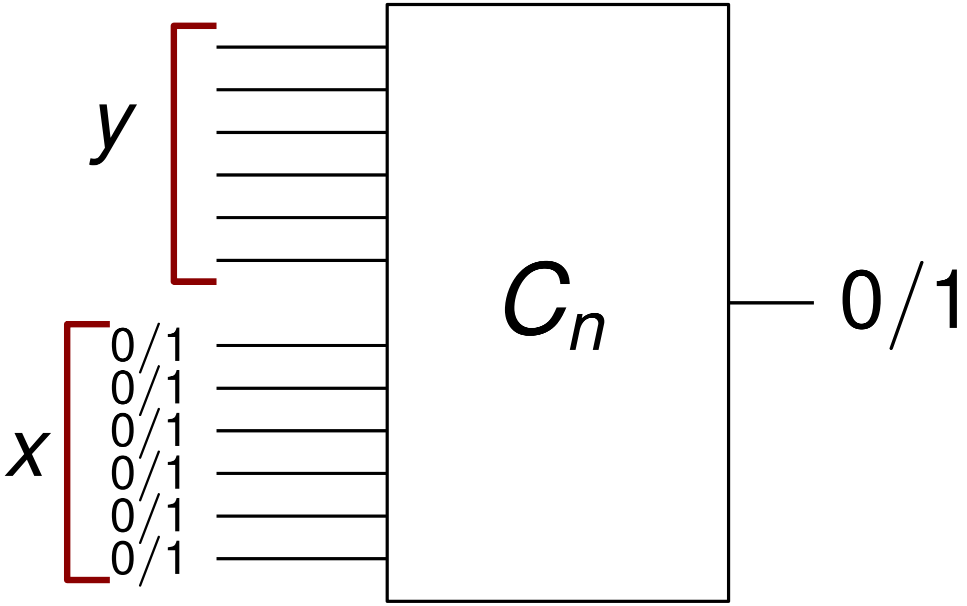

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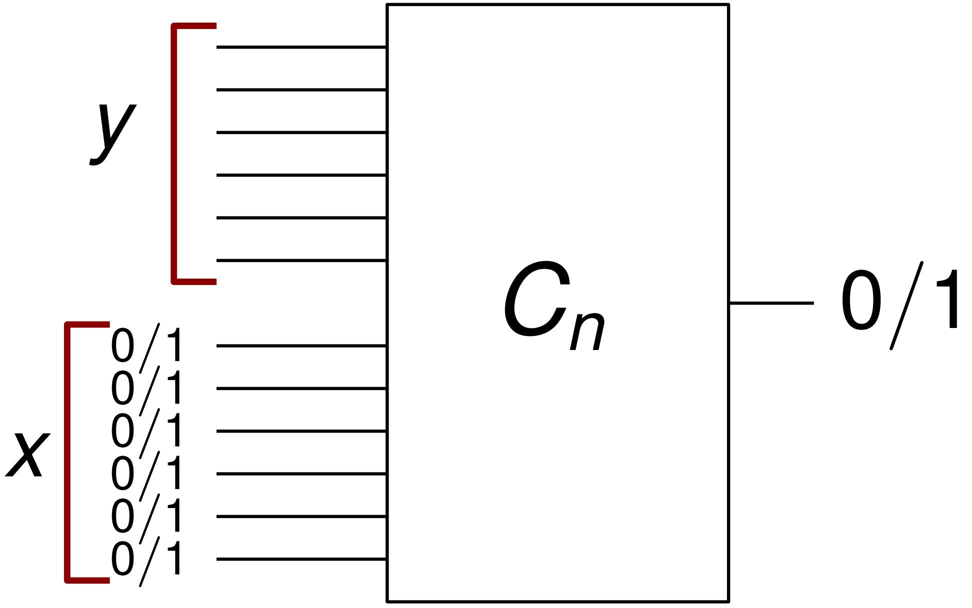

Is there a string y that causes this circuit to output 1?

Reduction: input x

- Use $|x| = n$ to compute C_n (uniformity)
- Convert C_n to a Boolean formula
- Add terms to hard-code input x and enforce output = 1.

Circuit to Boolean formula

Circuit C_n has gates $G_1, \ldots, G_m$, where $m = poly(n)$.

Add variables $g_1, \ldots, g_m$, one for each gate.

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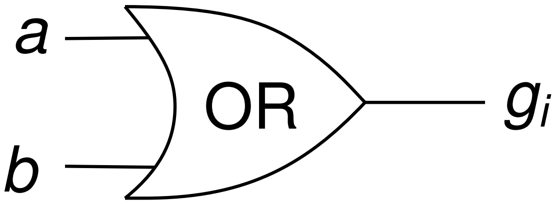
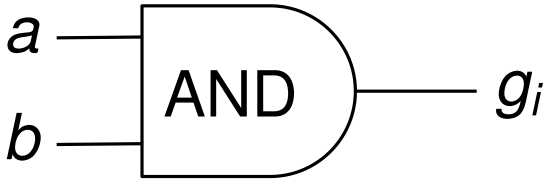
Add a clause for each gate:



$\Rightarrow \quad ((a \vee b) \leftrightarrow g_i)$



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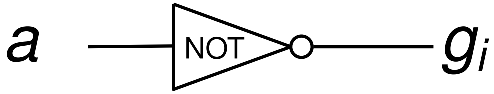

$\Rightarrow \quad (\neg a \leftrightarrow g_i)$

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Add a clause for each gate:

Hard-code x:

$x_i = 0 \quad \rightarrow$ add clause $(\neg x_i)$

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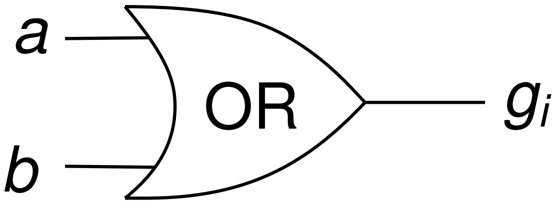
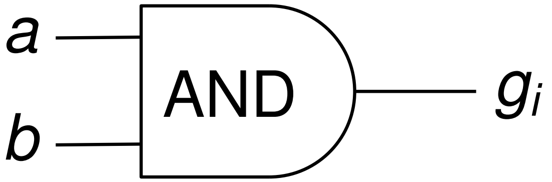


$\Rightarrow \quad ((a \vee b) \leftrightarrow g_i)$



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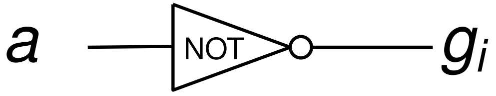

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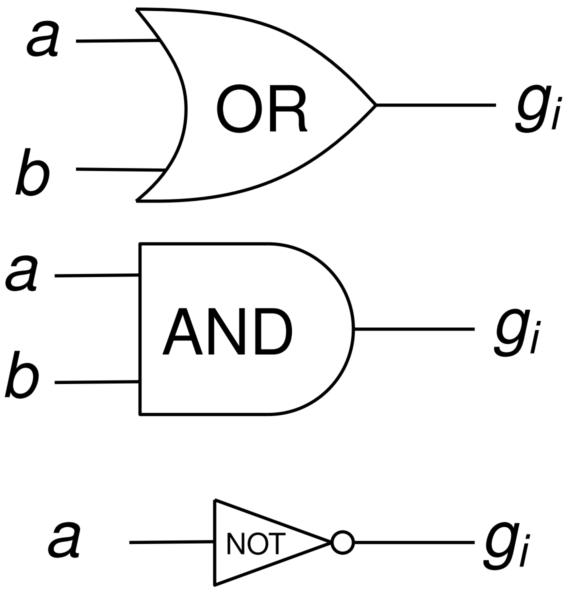
Circuit to Boolean formula

Circuit C_n has gates $G_1, \ldots, G_m$, where $m = poly(n)$.

Add variables $g_1, \ldots, g_m$, one for each gate.

Add a clause for each gate:



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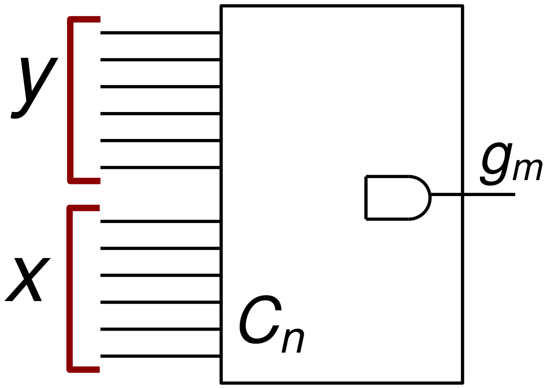

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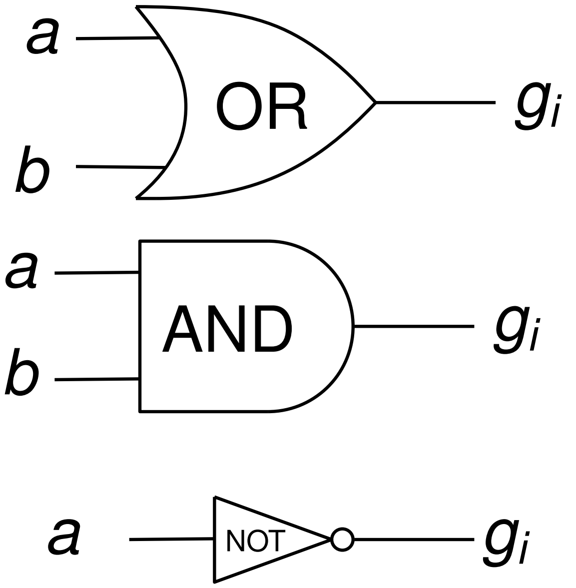

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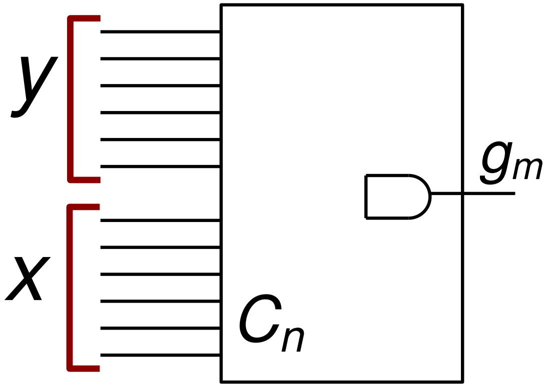

Boolean formula is the conjunction of all the clauses.

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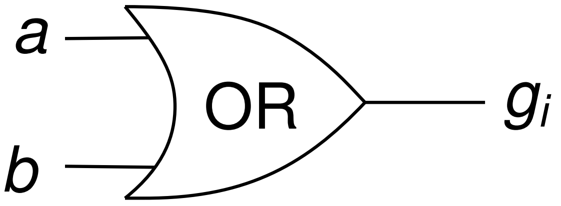

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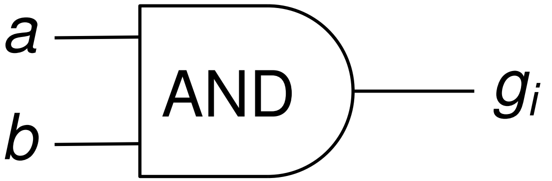

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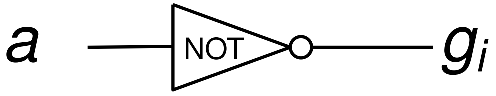

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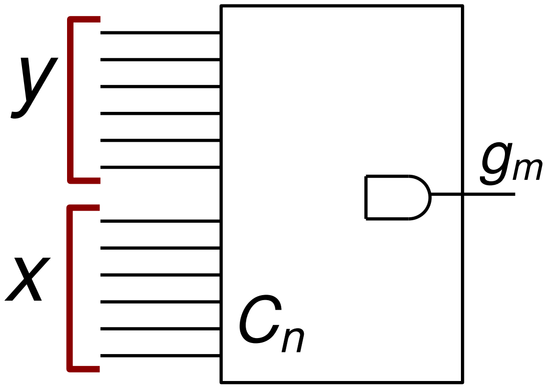

Boolean formula is the conjunction of all the clauses.

Can reduce to CNF or 3SAT form.

The class NP and Turing Machine Tableaus

NP

A problem is in NP if there is
a polynomial time algorithm A
that takes two inputs, x and y:

If $x \in L$, then there is a witness
y such that $A(x, y)$ accepts.

If $x \notin L$, then for every y,
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$|y| \leq \text{poly}(x)$

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Turing Machine that runs in time poly(n), where $|x| = n$

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Boolean Satisfiability is NP-hard

Start with a generic language L in NP

Is $x \in L$?

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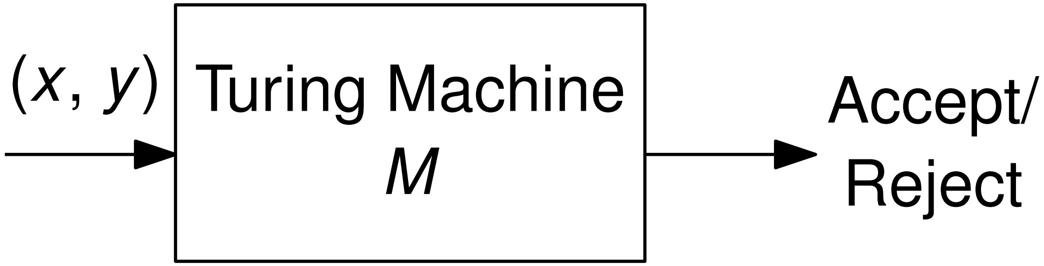

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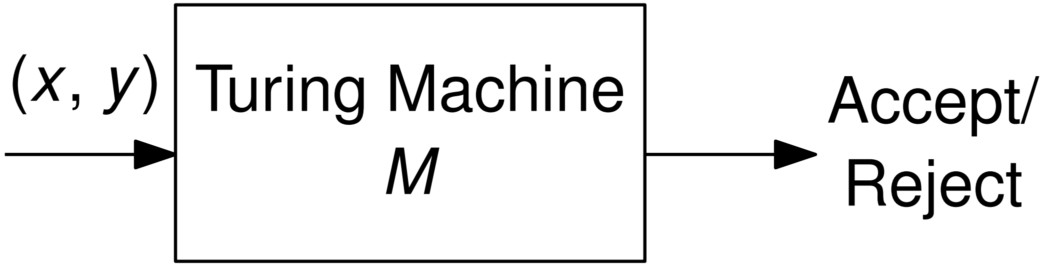

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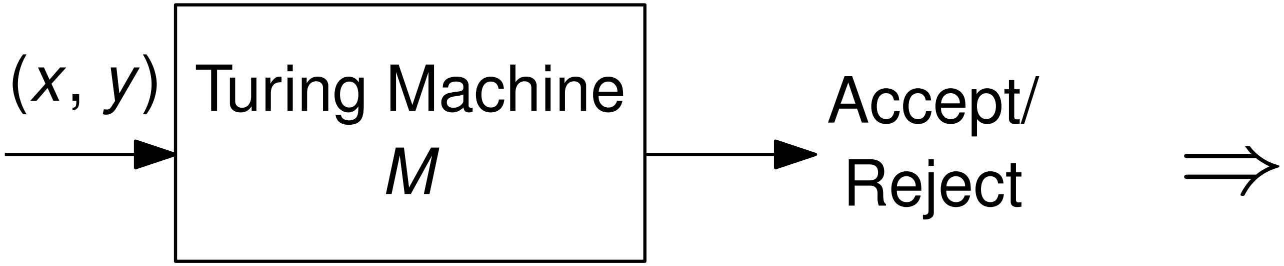


(x, y)

Turing Machine

M

Accept/

Reject

$\Rightarrow$

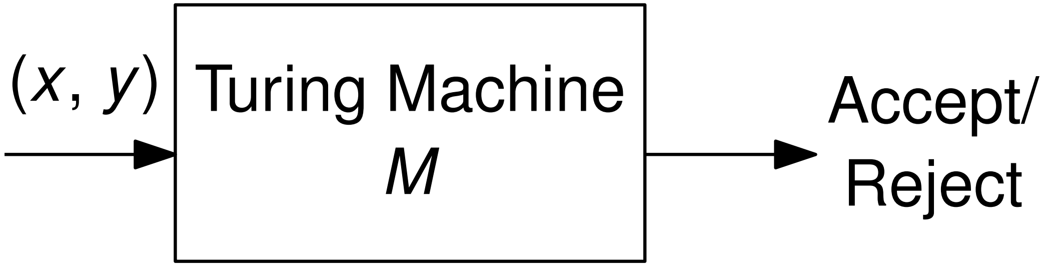
Boolean

Forumla:

$\Phi_x(y)$

Is there a string y that causes this Turing Machine to accept? $\Leftrightarrow$ Is $\Phi_x(y)$ satisfiable?

Turing Machine Tableau



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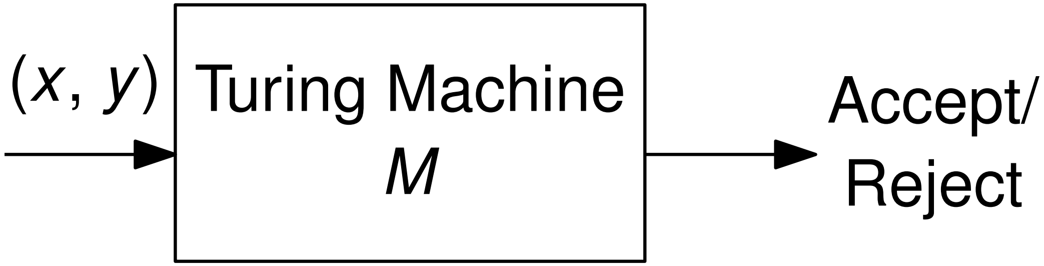
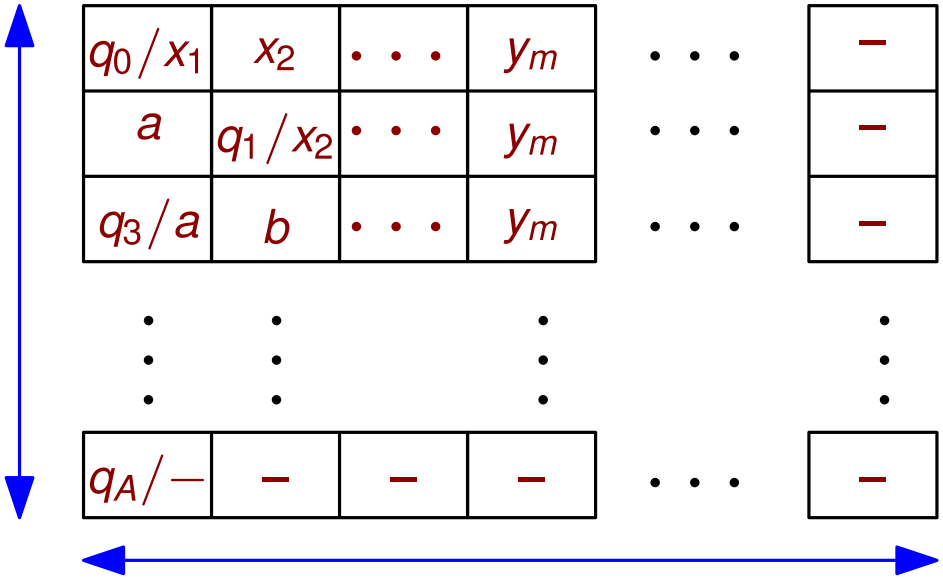


(x, y)

Turing Machine M

Accept/ Reject

TM Tableau:
Configurations written in a 2D array
for a Turing Machine M in input (x, y)



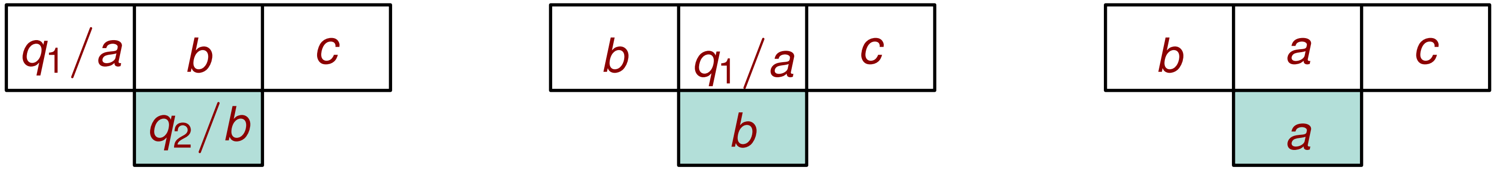
Height: running time $= n^c$.

q_0/x_1	x_2	$\cdots$	y_m	$\cdots$	$-$
a	q_1/x_2	$\cdots$	y_m	$\cdots$	$-$
q_3/a	b	$\cdots$	y_m	$\cdots$	$-$
$\vdots$	$\vdots$		$\vdots$		$\vdots$
$q_A/-$	$-$	$-$	$-$	$\cdots$	$-$

Width: space used $\leq n^c$

Turing Machine to Boolean formula

Contents of a cell determined by the three cells above it.



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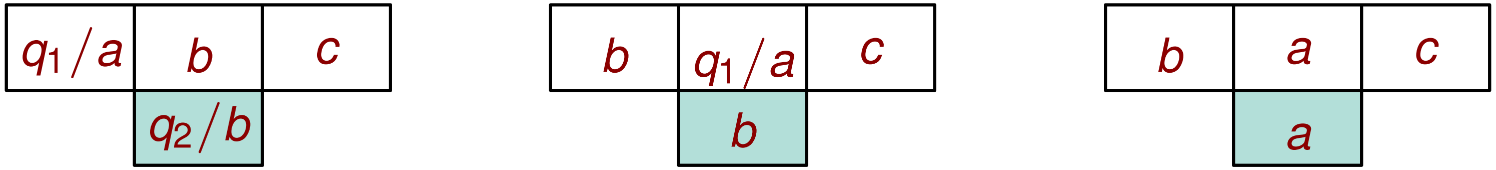
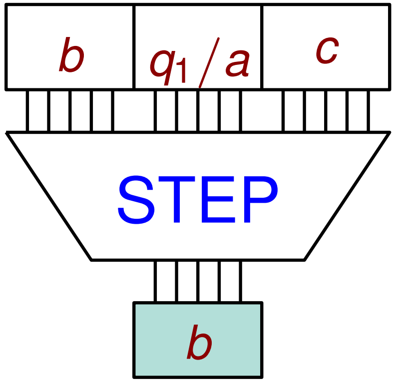


Can build Boolean circuit STEP

- input (binary encording of) 3 cells
- output (binary encording of) 1 cell

Circuit is constant size



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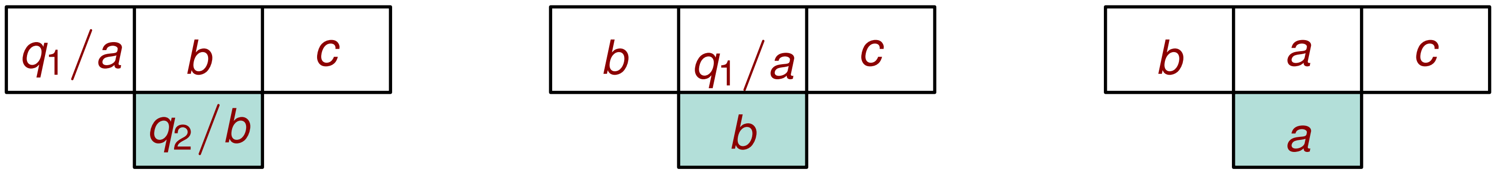

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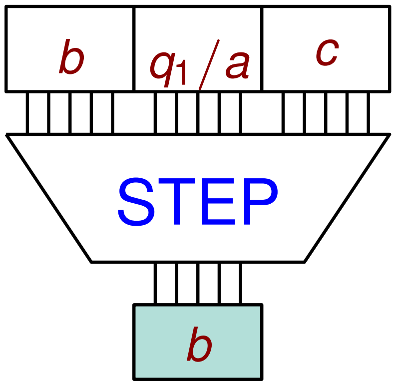
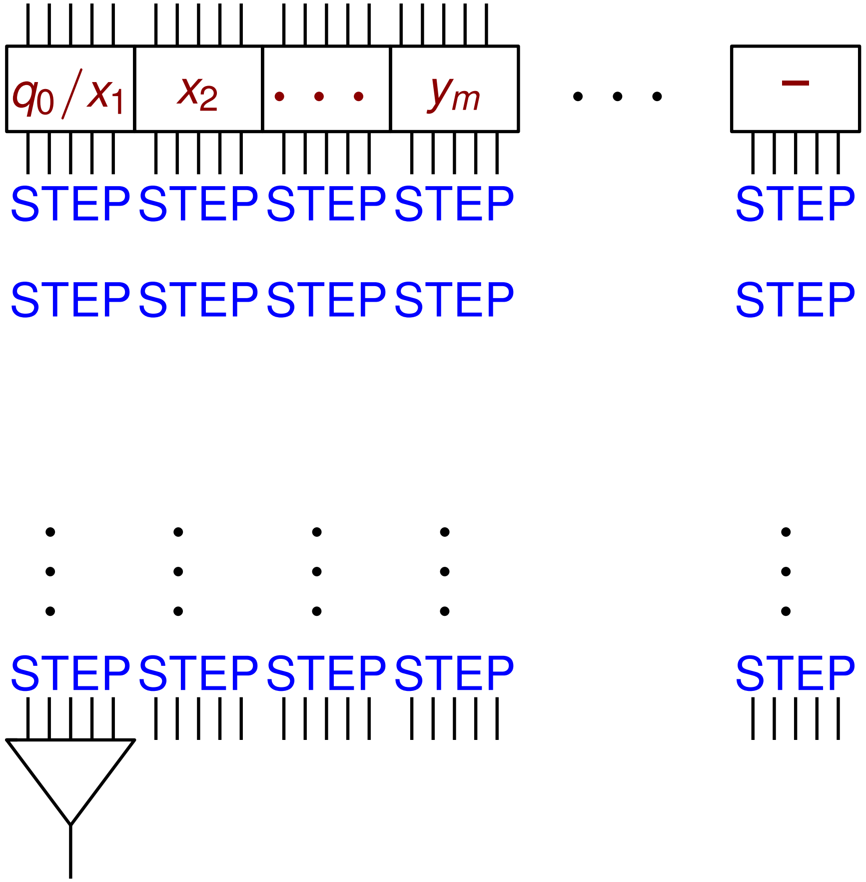


Each circuit can be converted to a Boolean formula
(set of Boolean constraints)

Turing Machine to Boolean formula



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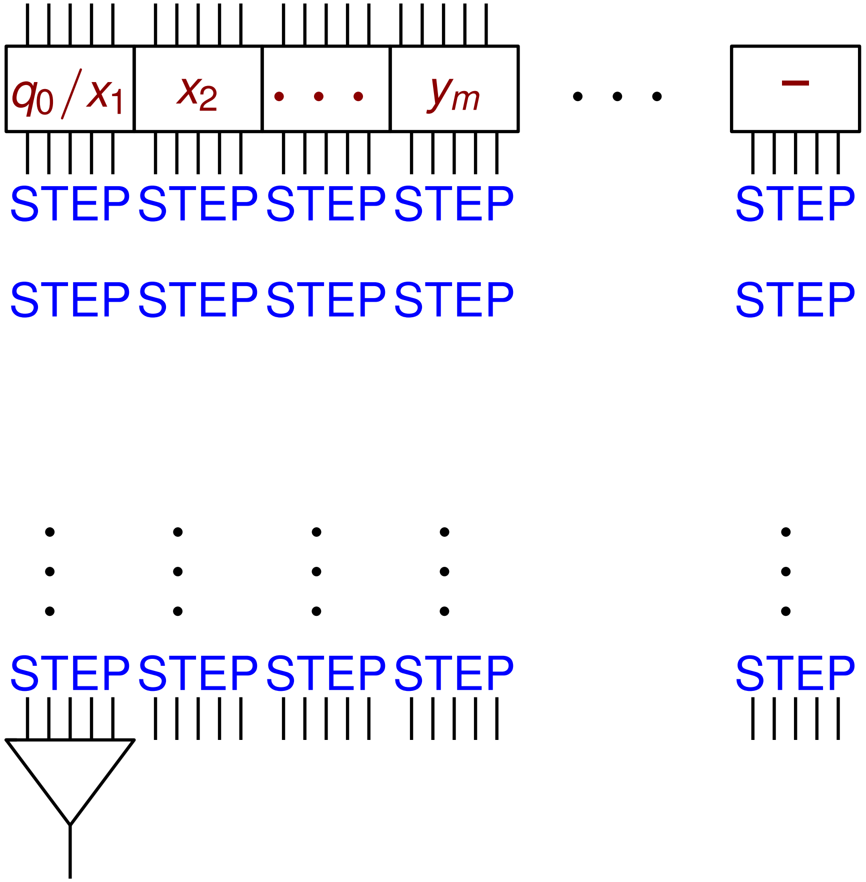

q_0 / x_1 x_2 . . . y_m . . . $-$

STEP STEP STEP STEP STEP

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Output 1 iff cell contains q_{ACC}

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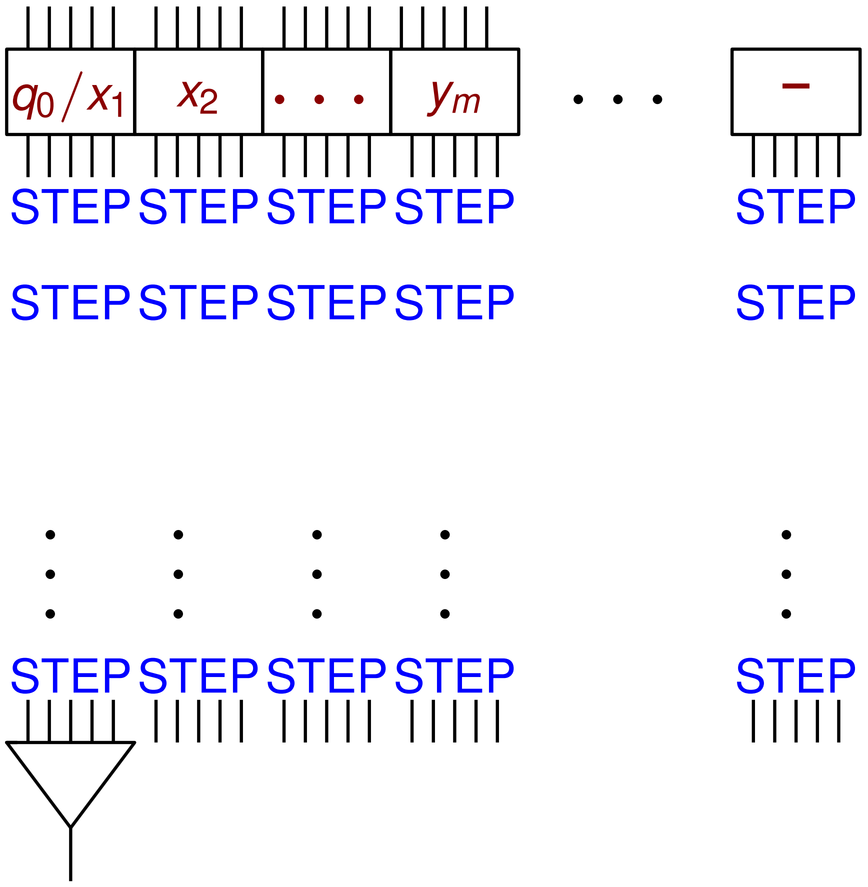

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Features we will keep for QMA

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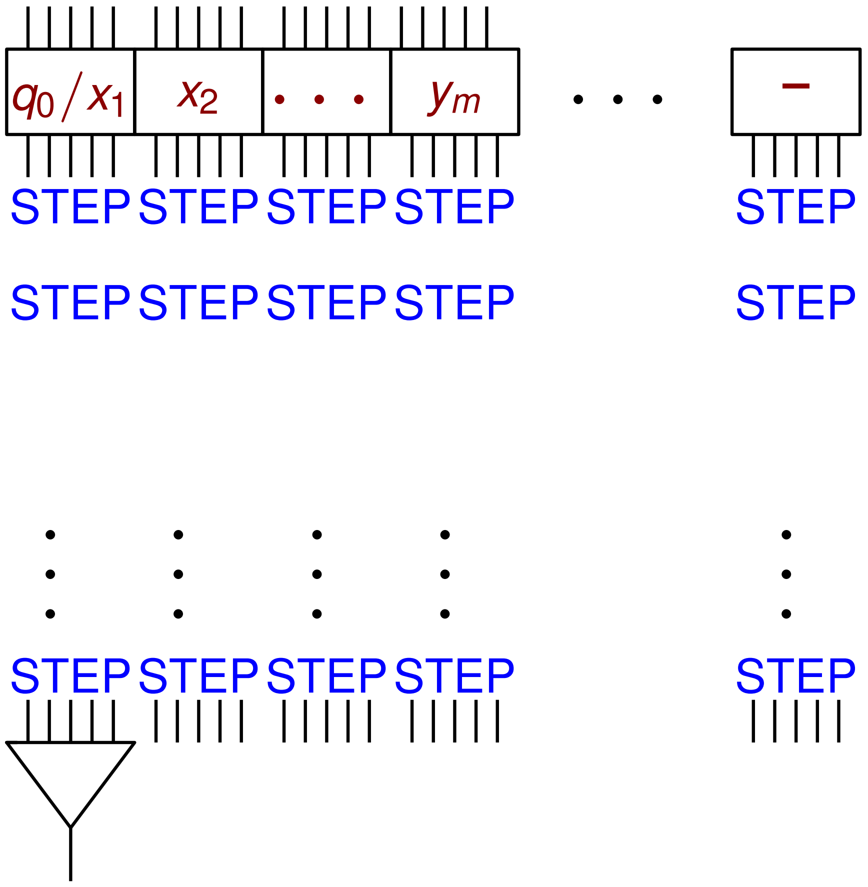

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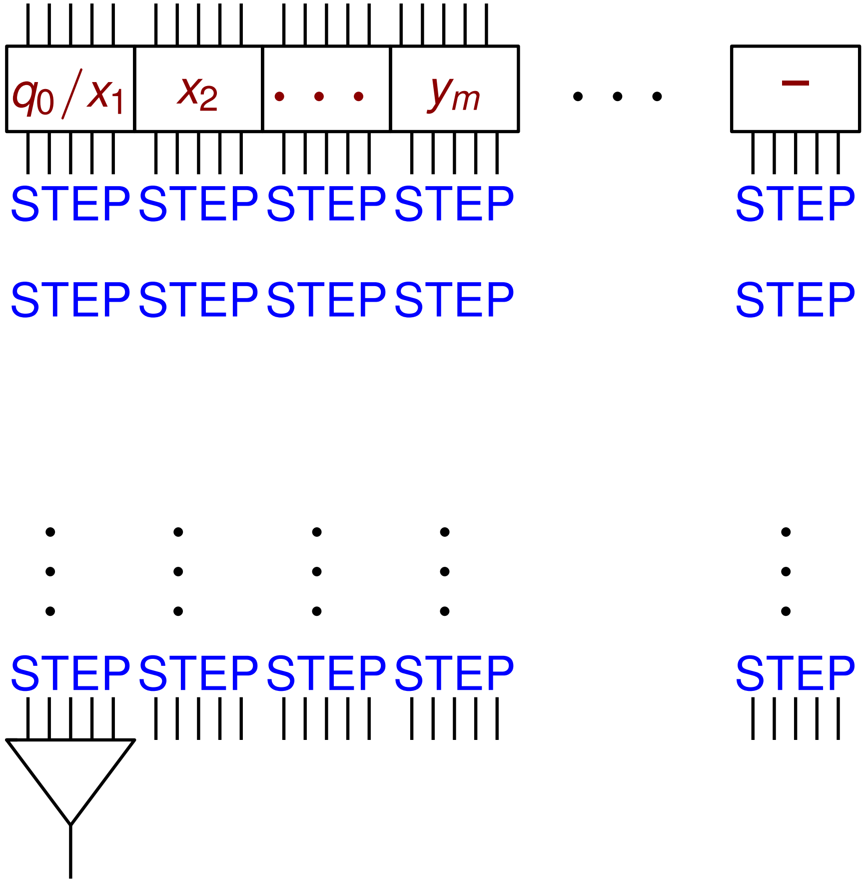

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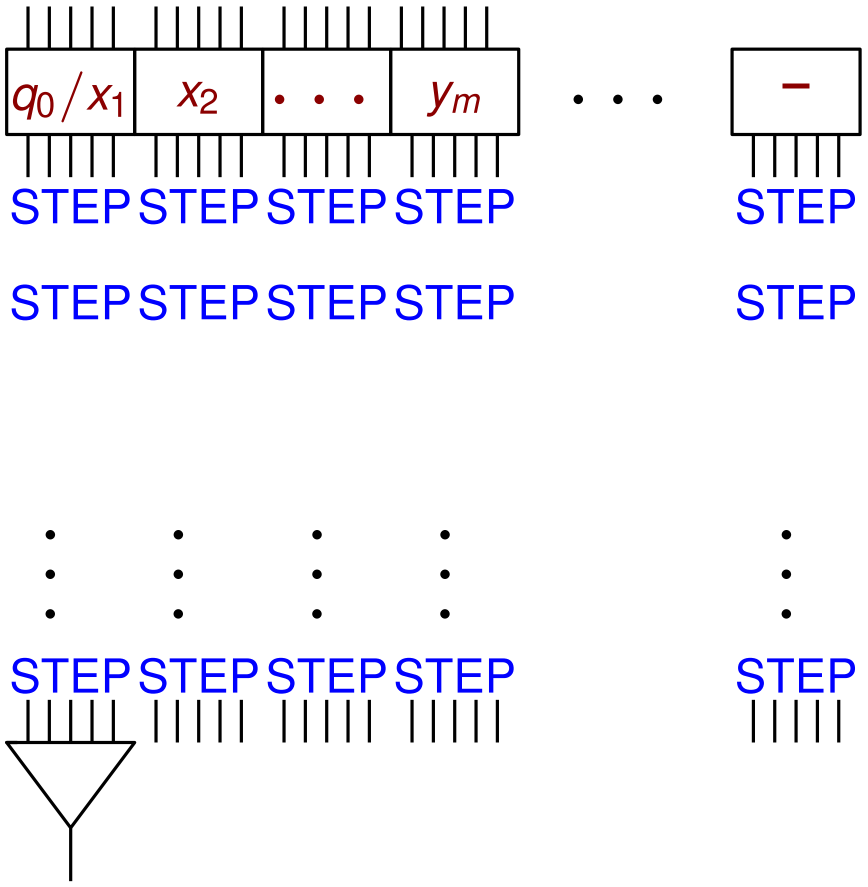

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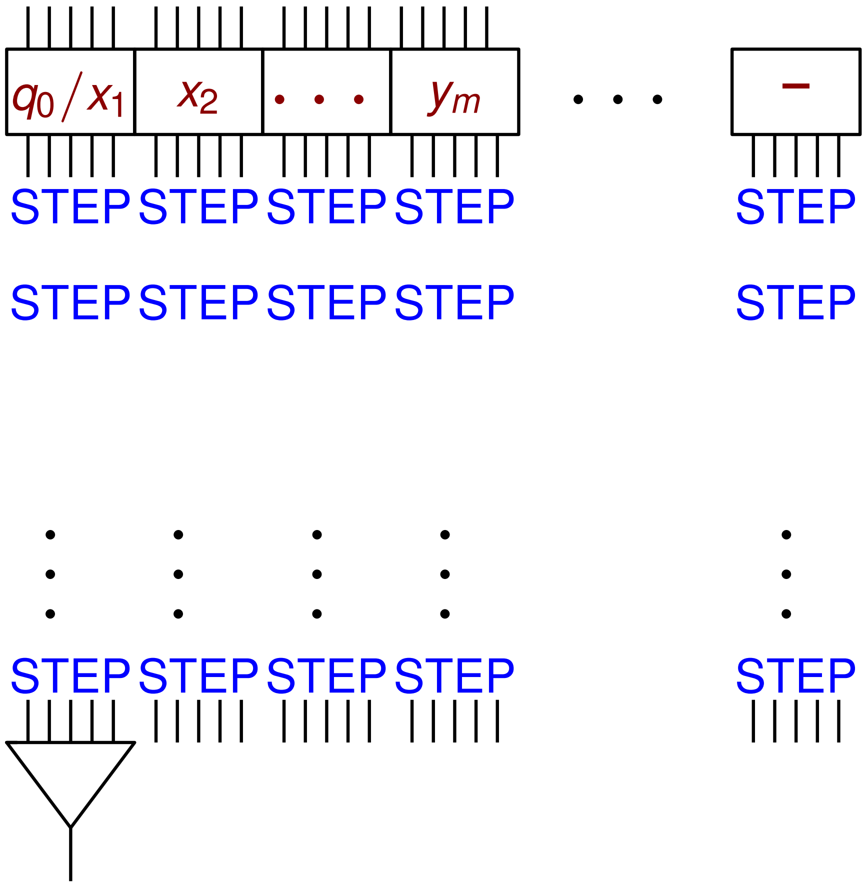

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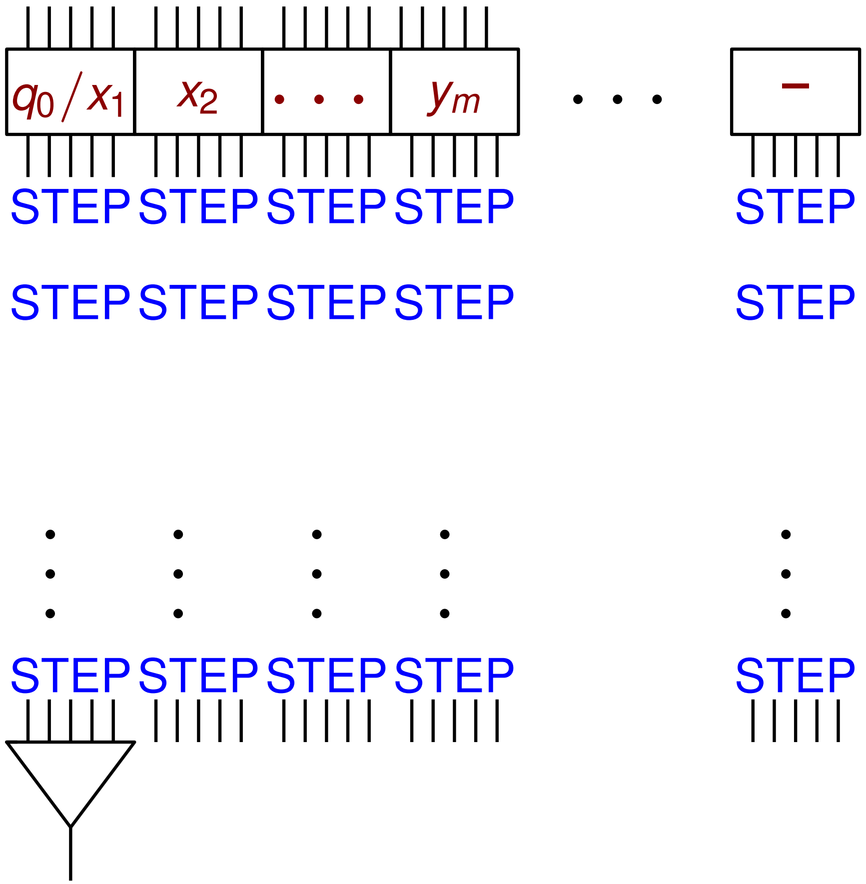

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On to Part II...